A METHOD FOR DESIGNING A COMPOUND BASED ON THE THREE DIMENSIONAL STRUCTURE OF PHOSPHOINOSITIDE DEPENDENT PROTEIN KINASE I (PDK1)

Cross-reference to Related Application

The present application is the US national phase under 35 USC 371 of International Application No. PCT/GB03/02509, filed June 9, 2003, and published in the English language as WO 03/104481.

Reference to Sequence Listing

The present application incorporates by reference the sequence listing submitted as an ASCII text filed via EFS-Web on January 18, 2010. The Sequence Listing is provided as a file entitled 8400121_1.txt, created on January 18, 2010, which is 4 Kb in size.

15 Field of the Invention

The present invention relates to protein kinase catalytic domain structures and mutants and screening assays making use thereof.

Background of the Invention

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) is a key protein kinase, regulating activity of a group of related protein kinases through phosphorylation. These kinases include isoforms of Protein Kinase B (also known as Akt) [Brazil and Hemmings, 2001, Scheid and Woodgett, 2001], p70 ribosomal S6 kinase (S6K) [Alessi et al.,1997, Volarevic and Thomas, 2001], p90 ribosomal S6 Kinase (RSK) [Frodin and Gammeltoft, 1999] and the serum and glucocorticoid induced-protein kinase (SGK) [Lang and Cohen, 2001]. These enzymes are stimulated by hormones and growth factors and phosphorylate regulatory proteins mediating the various physiological effects of these agonists.

PDK1 possesses an N-terminal kinase catalytic domain and a C-terminal pleckstrin homology (PH) domain [Alessi et al., 1997, Stephens et al., 1998]. PDK1 activates its substrates by phosphorylating these kinases at their activation loop (reviewed in [Alessi, 2001, Toker and Newton, 2000]). The phosphorylation of PKB by PDK1 is dependent upon prior activation of the phosphoinositide 3-kinase (PI-3-kinase) and the production of the second messenger, phosphatidylinositol 3,4,5-trisphosphate (PtdIns(3,4,5)P₃) which binds to the PH domains of PDK1 and PKB. This does not activate either PKB or PDK1 but instead recruits and co-localises these enzymes at the plasma membrane.

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Unlike PKB, the other PDK1 substrates described thus far do not interact with PtdIns(3,4,5)P₃ nor is the rate at which they are phosphorylated by PDK1 further enhanced by the binding of PDK1 to PtdIns(3,4,5)P₃. Instead the ability of PDK1 to phosphorylate S6K, SGK and RSK is promoted by phosphorylation of these enzymes at a residue located C-terminal to the kinase catalytic domain in a region known as the hydrophobic motif [Alessi et al., 1997,Kobayashi and Cohen, 1999, Pullen et al., 1998]. The kinases that phosphorylate the hydrophobic motif of S6K and SGK are unknown but as the phosphorylation of this residue *in vivo* is dependent on PI-3-kinase activation, the hydrophobic motif kinases and/or the hydrophobic motif phosphatases may be regulated by PtdIns(3,4,5)P₃. In the case of RSK isoforms, phosphorylation by the ERKI/ERK2 MAP kinases induce phosphorylation of the hydrophobic motif (reviewed in Frodin and Gammeltoft, 1999).

PDK1 belongs to the same subfamily of protein kinases as its substrates, termed the AGC protein kinases as they are related to the cAMP dependent protein kinase (PKA)/cGMP dependent protein kinase/Protein kinase C (PKC). PKA is the only AGC kinase whose crystal structure has been

solved. Like all protein kinases, its catalytic core possesses an N-terminal lobe consisting mainly of β-sheet and a predominantly α-helical Cterminal lobe [Taylor et al., 1992, Husen and Kuriyan, 2002]. The ATP binding site is located in between the 2 lobes [Johnson et al., 2001, Knighton et al., 1991]. At the very C-terminus, PKA possesses an extended loop that terminates in the sequence FXXF (SEQ ID NO:1) which resembles the first part of the hydrophobic motif phosphorylation site of S6K and SGK (FXXFS/TY, SEQ ID NO:2) in which the Ser/Thr is the phosphorylated residue [Biondi et al., 2000]. In the structure of PKA, the FXXF motif (SEO ID NO:1) is buried in a hydrophobic pocket in the small lobe of the PKA catalytic domain [Knighton et al., 1991] and mutation of either of the Phe residues drastically reduces PKA activity towards a peptide substrate [Etchebehere et al., 1997]. Unlike other AGC kinases, PDK1 does not possess a hydrophobic motif C-terminal to its catalytic domain. However, there is evidence that PDK1 possesses a hydrophobic pocket in the small lobe of its catalytic domain similar to that in PKA. We have biochemically demonstrated that the interaction of PDK1 with four of its substrates (S6K1, SGK1, PKZ and PKC related kinase-2 (PRK2)) is reduced or abolished by mutation of residues predicted to form part of this pocket [Balendran et al., 2000, Biondi et al., 2000]. Furthermore, mutation of a central residue in the predicted pocket, Leu 155, prevented PDK1 from phosphorylating and activating S6K1 and SGK1 without affecting its ability to phosphorylate either PKB or a short peptide substrate that encompasses the activation loop of PKB (T308tide) [Biondi et al., 2000]. The hydrophobic pocket on the kinase domain of PDK1 has been termed the "PIF-pocket" after the name of the first AGC-kinase hydrophobic motif-containing peptide (PDK1 Interacting Fragment) that was found to bind PDK1 [Balendran et al., 1999al. It has been suggested that the PIF-pocket in PDK1 functions as a docking site, enabling PDK1 to interact with some of its.physiological substrates. Furthermore, there is evidence that phosphorylation of the

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hydrophobic motif of S6K1, SGK and RSK2 [Balendran et al., 1999b,Biondi et al., 2001, Frodin et al., 2000] promotes the interaction of these enzymes with PDK1. These findings suggest that the PIF-pocket on PDK1 could contain a phosphate binding site promoting the binding of PDK1 to a subset of substrates (S6K, SGK and RSK) once these enzymes have been phosphorylated at their hydrophobic motif. This would result in a physiological phosphate dependent interaction. In addition there is evidence that occupancy of the PIF-pocket activates PDK1 as peptides that encompass the hydrophobic motif of PRK2 [Biondi et al., 2000] and RSK [Frodin et al., 2000] induce a 4-6-fold activation of PDK1.

Previous predicted structures PDK1 catalytic domain were obtained using homology modelling methods based upon structural information available from the catalytic domain of PKA (Biondi et al., 2000). These predictions of the PDK1 catalytic domain structure were thus biased towards the catalytic domain from which the structural information was obtained.

Summary of the Invention

We have determined a crystal structure for the kinase domain of the AGC family protein kinase PDK. The structure defines the PIF-pocket and reveals an adjacent possible phosphate binding site. Furthermore, we have performed structure-based mutagenesis and biochemical analysis which support the existence of such a phosphate-binding site. This may mediate the phosphate dependent docking interaction with substrates such as (for PDK1) S6K and SGK. We have used a novel algorithm to define the conformational state of the crystallised PDK1 relative to all the reported structures of PKA, which shows that while PDK1 has all the signs of being in an active form in the crystal, its overall conformation is in-between and 'open' and 'closed' state. We have also determined crystal structures for the kinase domain of PDK1 in complex with modulators of PDK1 activity.

On the basis of this work we provide drug screening methods and mutated protein kinase molecules (which are useful in, for example, drug screening methods).

a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

Brief Description of the Drawings

Figure 1 provides an overview of the PDK1 structure.

Figures 2A and 2B show the PIF-pocket.

Figure 3 shows a structure-based sequence alignment

Figures 4A-C show PDK1 binding & activation studies.

Figures 5A and 5B show interactions of regulatory phosphates with the αC

helix

Figures 6A and 6B show essential dynamics.

Figure 7 shows alignment of AGC protein kinase family members.

Figure 8 shows staurosporine and UCN-01 electron density.

Figure 9 shows details of the inhibitor binding sites.

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Detailed Description of the Invention

The term PDK1 as used herein includes a polypeptide (a PDK1 polypeptide) comprising the amino acid sequence identified as PDK1 in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776-789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714, or a variant, fragment, fusion or derivative thereof, or a fusion of a said variant or fragment or derivative, for example as described in WO98/41638, incorporated herein by reference. It is preferred that the said PDK1 polypeptide is a protein kinase. It is preferred that the said PDK1 polypeptide is a protein kinase that is capable of phosphorylating a threonine residue that lies in a Thr-Phe-Cys-Gly-Thr-Xaa-Glu-Leu consensus motif (where the underlined Thr corresponds to the threonine that is phosphorylated by PDK1 and Xaa is a variable residue. SEQ ID NO:9), and preferably that is capable of phosphorylating PKB, for example PKBa, at residue Thr308. The rate at which the said PDK1 polypeptide is capable of phosphorylating a threonine residue as described above may be increased in the presence of PtdIns(3,4,5)P3 or PtdIns(3,4)P2 but it will be appreciated that this is not essential. The said polypeptide may be capable of phosphorylating the equivalent residues to Thr308 of PKBa on PKC isoforms (LeGood et al (1998) Science 281: 2042-2045; et al (1998) Curr. Biol. 8: 1069-1077; Dutil et al (1998) Curr. Biol. 8:1366-1375), p70 S6 kinase (Alessi et al (1998) Curr. Biol. 8: 69-81; Pullen et al (1998) Science 279, 707-710), SGK (sequence given in Webster et al. (1993) Mol. Cell. Biol. 13, 1031-2040; equivalent residues identified in US application no 112217 filed on 14 December 1998; GB 9919676.8, filed on 19 August 1999, and Kobayashi & Cohen (1999)) and PKA (Cheng et al. (1998) Proc. Natl. Acad. Sci. USA 95: 9849-9854). It may further be preferred that the substrate specificity and/or other characteristics of the said PDK1 polypeptide in vitro may be substantially as reported in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714.

We have found that a fragment of PDK1 consisting essentially of residues equivalent to residues 51 to 359 of full length human PDK1 is particularly beneficial for determining a structure for the catalytic domain of PDK1. This fragment has, for example, protein kinase activity and surprisingly beneficial solubility and stability characteristics which make it particularly suitable for structural studies, for example formation of crystals which may be analysed by X-ray crystallography methods. Other fragments of PDK1 were surprisingly found to be unsuitable for crystallisation, as discussed in Example 5.

It is particularly preferred that the structure is one determined for the fragment consisting of residues 51 to 359 of full length human PDK1. The fragment may comprise an N-terminal or C-terminal fusion polypeptide (ie amino acid sequence not derived from PDK1), though this is preferably of less than or equal to about 10, 5, 4, 3, 2 or 1 amino acids. For example, it is particularly preferred that the structure is one determined for a polypeptide consisting residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro (or less preferably other sequence forming part of a protease cleavage site) preceding the methionine corresponding to Met51 of human PDK1. A further preferred structure is one determined for the fragment consisting essentially of residues 71 to 359 of full length human PDK1 (or residues equivalent thereto), which also has protein kinase activity.

It is particularly preferred that the structure is one determinable by a method as described in Example 1, for example a structure obtainable by X-ray analysis from a crystal obtainable using a mother liquor solution comprising ammonium sulphate, preferably between 1.8 and 2.2M. It is particularly preferred that the mother liquor solution is of pH 7 to 9, preferably 7 to 8.5, most preferably pH8.5, and comprises ammonium sulphate and preferably ATP. Crystals may form in the absence of ATP but better crystals may be obtained in the presence of ATP. Preferably the crystal is obtainable using a mother liquor solution containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP. Further preferred details of the crystallisation and X-ray analysis are described in Example 1, for example as partially summarised in Table 1 (shown in Example 1).

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It is particularly preferred that the structure is that represented by the structure co-ordinates shown in Examples 2, 3 or 4, or a structure based or modelled on such a structure or co-ordinates. The co-ordinates shown in Example 2 are for the PDK1 fragment (SEQ ID NO:102) with all alternate side chains. The co-ordinates shown in Example 3 are for the PDK1 fragment (SEQ ID NO:102) without alternate side chains. The co-ordinates shown in Example 4 are for the dimer of the PDK1 fragment (SEQ ID NO:102), without alternate side chains; chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

The structure may be one determined following crystallisation in the presence of a known or potential interactor with PDK1 or modulator of PDK1 activity (as discussed further below), for example a known or potential inhibitor of PDK1 activity. For example, the structure may be one determined following crystallisation in the presence of a known protein kinase inhibitor, for example an inhibitor that binds at the ATP binding site, for example an ATP-competitive inhibitor, for example staurosporine or a staurosporine derivative, for example UCN-01. Examples of such crystallisation techniques and analysis are given in Example 6, and

examples of co-ordinates are given in Examples 7 and 8. Example 7 represents the co-ordinates of PDK1 fragment (SEQ ID NO:102) co-crystallised with Staurosporine, whereas in Example 8, the co-ordinates of PDK1 fragment (SEQ ID NO:102) co-crystallised with UCN-01.

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It will be appreciated that some variation in crystallisation conditions (for example different mother liquors) may be required for co-crystallisation with different molecules. Techniques for investigating suitable crystallisation conditions in each case will be well known to those skilled in the art

A further aspect of the invention provides a crystalline form of a polypeptide as defined in any of the preceding aspects of the invention, for example a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof; a polypeptide consisting of residues 51 to 359 of full length human PDK1 or a fusion thereof; a polypeptide consisting of residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro preceding the methionine corresponding to Met51 of human PDK1; a polypeptide consisting of residues 71 to 359 of full length human PDK1 or a fusion thereof.

The crystalline form may further comprise co-crystallised molecule, for example a known or potential interactor with PDK1 or modulator of PDK1 activity, or a test compound whose properties vis a vis PDK1 may not be known. For example, the co-crystallised molecule, for example test compound, may be a molecule that is known to modulate protein kinase activity, or may already be known to modulate PDK1 protein kinase activity. For example, the co-crystallised molecule may be staurosporine,

the staurosporine derivative UCN-01 (7-hydroxyl staurosporine) or other staurosporine derivative.

Such co-crystallisation and structures determined from co-crystallised molecules may be useful in molecular modelling and in determining features of the polypeptide and compound that are important for interaction. This may be useful in designing or selecting further test compounds, for example as discussed in Example 6.

In one embodiment it is preferred that the modelled molecule is predicted to bind to a region of the structure termed the "PIF binding pocket", the "phosphate binding pocket" and/or the α C helix (residues equivalent to 123-136 of full length human PDK1), particularly the residue equivalent to Arg 131 of full length human PDK1, or interacting regions. As discussed in Example 1, the PIF binding pocket is considered to be formed by residues including Lys115, Ile118, Ile119 on the α B helix, Val124, Val127 on the α C helix and Leu 155 on β -sheet 5. The phosphate binding pocket is considered to be formed by residues including Lys76, Arg 131, Thr 148 and Gln150. Residues of the α C helix that are considered to interact either with phosphate bound in the phosphate binding site or intermolecularly with phosphorylated Ser241 of PDK1 include Arg131 (phosphate binding site) and Arg 129 and His126 (phosphorylated Ser241). Glu 130 is involved in binding the α -phosphate of the bound ATP, and Val124 and Val127 form part of the PIF binding pocket, as discussed in Example 1.

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It is preferred that the compound is for modulating the protein kinase activity of PDK1. The protein kinase activity of PDK1 that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu ("PDK1"

activity, SEQ ID NO:9). Alternatively or in addition, the modulated activity may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Phe-Xaa-Xaa-Phe-Ser/Thr-Phe/Tyr ("PDK2" activity. SEQ ID NO:11). The substrate polypeptide may be, for example, a PKB, SGK, p70 S6 kinase, PKC or (in relation only to phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu (SEQ ID NO:9) PKA polypeptide. The modulated protein kinase activity may be towards PKB or other PHdomain-comprising/phosphoinositide-binding substrate of PDK1; or SGK, S6K or other substrate of PDK1 whose phosphorylation by PDK1 is promoted by phosphorylation of the substrate on the Ser/Thr of the "hydrophobic motif" FXXFS/TY (SEO ID NO:2); or an artificial substrate such as T308tide (which comprises the sequence of PKB which is phosphorylated by PDK1) or PDKtide (which comprises the sequence of PKB which is phosphorylated by PDK1 (eg T308tide) fused to a sequence mimicking a phosphorylated hydrophobic motif ie FXXFZY (SEQ ID NO: 2), in which Z is a negatively charged (for example acidic) residue (eg PIFtide)). Such substrates for PDK1 are discussed, for example, in WO 01/44497. Other activities of PDK1 that may be modulated include interactions with other polypeptides or phosphoinositides and/or intramolecular interactions.

It is preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of the PDK1 is a three-dimensional structure of at least a part of the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, and a compound that is predicted to interact with the said PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1 is selected. Alternatively, the compound may bind to a portion of said PDK1 polypeptide that is not the PIF binding pocket, the phosphate

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binding pocket and/or the α C helix, or interacting regions of PDK1, for example so as to interfere with the binding of the ATP or substrate polypeptide or their access to the catalytic site. In a still further example, the compound may bind to a portion of PDK1 so as to decrease said polypeptide's activity by an allosteric effect. This allosteric effect may be an allosteric effect that is involved in the natural regulation of PDK1's activity.

It is further preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure of the part of the protein kinase catalytic domain of PDK1 that is defined by residues Lys115, Ile118, Ile119 (on the αB helix), Val124, Val127 (on the αC helix) and Leu 155 (on β -sheet 50 and/or residues Lys76, Arg 131, Thr 148 and Gln150 and/or residues Arg131, Arg 129, His126, Glu 130 of full-length human PDK1 and a compound that is predicted to interact with the said part of the protein kinase catalytic domain is selected.

For example, it is preferred if the portions of the structure of PDK1 shown in Figures 1 and 2 as forming the PIF binding pocket and/or phosphate binding pocket and/or αC helix interactions (for example with phosphoserine241) are compared with the structure of the candidate compound.

25 A further aspect of the invention provides a method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase, wherein a three-dimensional structure of a compound is compared with a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, is selected.

The three-dimensional structure of a compound may be compared with the three-dimensional structure of the hydrophobic and/or phosphate binding pocket and/or αC helix or region interacting therewith, as appropriate. A compound that can interact with the hydrophobic pocket and/or phosphate binding pocket, in particular residues noted above as defining such regions, in a similar manner (for example similar separation and/or type of interaction ie hydrophobic or ionic, and/or similar cumulative energy of interaction) to an interacting polypeptide such as S6K-pHM may be selected. Methods of assessing the interaction are well known to those skilled in the art and are discussed further below.

The three-dimensional structures that are compared may be, as appropriate, predicted or modelled three-dimensional structures (for example on the basis of a PDK1 structure as referred to above, for example as represented by the co-ordinates given in Examples 2, 3 or 4 or 6 or 7) or may be three-dimensional structures that have been determined, for example by

techniques such as X-ray crystallography, as well known to those skilled in the art. The three-dimensional structures may be displayed by a computer in a two-dimensional form, for example on a computer screen. The comparison may be performed using such two-dimensional displays.

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The following relate to molecular modelling techniques: Blundell *et al* (1996) Stucture-based drug design *Nature* **384**, 23-26; Bohm (1996) Computational tools for structure-based ligand design *Prog Biophys Mol Biol* **66(3)**, 197-210; Cohen *et al* (1990) *J Med Chem* **33**, 883-894; Navia *et al* (1992) *Curr Opin Struct Biol* **2**, 202-210.

The following computer programs, for example, may be useful in carrying out the method of this aspect of the invention: GRID (Goodford (1985) J Med Chem 28, 849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al (1991) Proteins: Structure, Function and Genetics 11, 29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al (1990) Proteins: Structure, Function and Genetics 8, 195-202; available from Scripps Research Institute, La Jolla, CA); DOCK (Kuntz et al (1982) J Mol Biol 161, 269-288; available from the University of California, San Francisco, CA); LUDI (Bohm (1992) J Comp Aid Molec Design 6, 61-78; available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al (1991) Tetrahedron 47, 8985; available from Molecular Simulations, Burlington, MA); LeapFrog (available from Tripos Associates, St Louis, MO); Gaussian 92, for example revision C (MJ Frisch, Gaussian, Inc., Pittsburgh, PA @1992); AMBER, version 4.0 (PA Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA ©1994); and Insight II/Discover (Biosym Technologies Inc., San Diego, CA ©1994). Programs may be run on, for example, a Silicon

Graphics™ workstation, Indigo²™ or IBM RISC/6000™ workstation model 550.

Several *in silico* methods could be employed, for example, via a substructure search for new ligands using programmes such as CHEM DRAW or CHEM FINDER. The basic structure of the natural ligand (for example a phosphorylated hydrophobic motif peptide such as S6K-pHM) capable of binding to PDK1 (or other protein kinase) is taken (or predicted) and various structural features of it (for example the hydrophobic and negatively charged entities) are submitted to a programme which will searches a set of chemical company catalogues for chemicals containing this substructure.

These compounds are then screened by eye for groups that could not interact with the PIF/phosphate binding pockets (or the αC residues/interacting region) because, for example, they are too large or have steric or charge hindrance, and those are discarded. The remaining chemicals are submitted to a PRODRG server and topologies/co-ordinates for these chemicals are created. These chemicals are modelled into the structure, from which chemicals that are possibly able to bind to the PIF/phosphate binding site domain/ αC helix/interacting region are selected. Further details of the PRODRG programme are available <u>in</u> the art, for example, from Daan van Aalten Laboratory.

These compounds may then be ordered or synthesised and assessed, for one or more of ability to bind to and/or modulate PDK1 (or other protein kinase) activity. The compounds may be crystallised with the PDK1 or other protein kinase protein and the structure of any complex determined, as illustrated in Examples 6 to 8.

An alternative approach is to use PRODRG: a tool for generating GROMOS/MOL2/WHATIF topologies and hydrogen atom positions from small molecule PDB files. We take the natural ligand and computationally vary all possible groups at each site on the ligand, with a variety of new groups while the protein co-ordinates and the ligand back-bone co-ordinates remain fixed the results can then be screened for hindrance and repulsion, and the molecules are obtained either through catalogues or made.

As noted above, the selected or designed compound may be synthesised (if not already synthesised) or purified and tested for its effect on the relevant hydrophobic/phosphate pocket-containing protein kinase, for example its effect on the protein kinase activity. The compound may be tested in a screening method of the invention or other screening method. The compound may be formulated for pharmaceutical use, for example for use in *in vivo* trials in animals or humans, or for use in agriculture, for example as an antifungal agent.

It may be useful to analyse a protein kinase structure (for example a structure determined or predicted for a complex of the protein kinase with a binding partner) in order to determine the activation state of the structure. This may be useful in further modelling binding of the binding partner to the protein kinase in other activation states, and in predicting how the binding partner may affect the activation state of the protein kinase or compete with other potential binding partners. It may also be useful in designing and assessing derivatives of the binding partner.

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Thus, a further aspect of the invention provides a method for assessing the activation state of a structure for a protein kinase, wherein the structure is analysed using principle component analysis of the structure co-ordinates. The method may further comprise the step of classifying the activation state

of the structure as "open", "closed" or "intermediate". Details of the analysis, which involves the generation of eigenvectors and associated eigenvalues are given in Example 1. The analysis makes use of techniques described in Amadei et al (1993) Essential dynamics of proteins. Proteins 17, 412-425.

The hydrophobic/phosphate pocket-containing protein kinase may be PDK1. Alternatively, it may be an isoform of Serum and Glucocorticoid stimulated protein kinase (SGK), Protein Kinase B (PKB), p70 S6 kinase, p90 RSK, PKC isoforms (for example PKCα, PKCδ, PKCζ), PRK1, PRK2, MSK1 or MSK2. Hydrophobic/phosphate pocket-containing protein kinases and their EMBL database accession numbers are listed in Table I. Sequences considered to form the phosphate binding pocket from representative hydrophobic/phosphate pocket-containing protein kinases are shown in Figure 5. All AGC family protein kinases other than PKA may be hydrophobic/phosphate pocket-containing protein kinases, as defined above. In addition to the protein kinases shown in Figure 7, rhodopsin and G-protein coupled receptor protein kinases, for example, may possibly also have a hydrophobic/phosphate pocket as defined above.

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The terms SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, for example, as used herein include a polypeptide (a SGK, PKB, PKA, p70S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 polypeptide) comprising the amino acid sequence identified as a SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, respectively, in the relevant EMBL database records indicated in Table 2.

Table 2

	Loop	Motif	number
consensus:	$\underline{T}FCGTxxYxAPD$	FxxF <u>S</u> Y	
	(SEQ ID NO:41)	(SEQ ID NO:42)	
	L E	Y <u>T</u> F	
ΡΚΒα	$\underline{\mathbf{T}}$ FCGTPEYLAPE	FPQF <u>S</u> Y	(Y15056)
	(SEQ ID NO:45)	(SEQ ID NO:46)	
РКВβ	$\underline{T}FCGTPEYLAPE$	FPQF <u>S</u> Y	(P31751)
	(SEQ ID NO:47)	(SEQ ID NO:48)	
ΡΚΒγ	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	FPQF <u>S</u> Y	(AF135794)
	(SEQ ID NO:49)	(SEQ ID NO:50)	
SGK1	$\underline{T}FCGTPEYLAPE$	FLGF <u>S</u> Y	(AAD41091)
	(SEQ ID NO:51)	(SEQ ID NO:52)	
SGK2	$\underline{T}FCGTPEYLAPE$	flgf <u>s</u> y	(AF169034)
	(SEQ ID NO:53)	(SEQ ID NO:54)	
SGK3	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	FLGF <u>S</u> Y	(AF169035)
	(SEQ ID NO:55)	(SEQ ID NO:56)	
ΡΚCα	$\underline{T}FCGTPDYIAPE$	FEGF <u>S</u> Y	(4506067)
	(SEQ ID NO:57)	(SEQ ID NO:58)	
РКСВІ	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	fagf <u>s</u> y	(4506069)
	(SEQ ID NO:59)	(SEQ ID NO:60)	
РКСВІІ	TFCGTPDYIAPE	fegf <u>s</u> f	(P05127)
	(SEQ ID NO:61)	(SEQ ID NO:62)	
ΡΚСγ	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	FGGF <u>T</u> Y	(P05129)
	(SEQ ID NO:63)	(SEQ ID NO:64)	
ΡΚCδ	TFCGTPDYIAPE	FAGF <u>S</u> F	(5453970)
	(SEQ ID NO:65)	(SEQ ID NO:66)	
ΡCΚζ	TFCGTPNYIAPE	FEGFEY	(4506079)
	(SEQ ID NO:67)	(SEQ ID NO:68)	
PKCι	$\underline{T}FCGTPNYIAPE$	FEGFEY	(4506071)
	(SEQ ID NO:69)	(SEQ ID NO:68)	

PRK1	$\underline{T}_{FCGTPEFLAPE}$	FLDFDF	(AAC50209)
	(SEQ ID NO:71)	(SEQ ID NO:72)	
PRK2	$\underline{T}FCGTPEFLAPE$	FRDFDY	(AAC50208)
	(SEQ ID NO:73)	(SEQ ID NO:74)	
p70-S6Kα	\underline{T} FCGTIEYMAPE	FLGF <u>T</u> Y	(AAA36410)
	(SEQ ID NO:75)	(SEQ ID NO:76)	
p70-S6Kβ	$\underline{\mathtt{T}}\mathtt{FCGTIEYMAPE}$	FLGF <u>T</u> Y	(4506739)
	(SEQ ID NO:77)	(SEQ ID NO:78)	
p90-RSK1	\underline{s} FCGTVEYMAPE	FRGF <u>S</u> F	(138556)
	(SEQ ID NO:79)	(SEQ ID NO:80)	
p90-RSK2	SFCGTVEYMAPE	FRDFSF	(P51812)
p		_	,
p	(SEQ ID NO:81)	_	,
•	_	(SEQ ID NO:82)	(CAA59427)
•	(SEQ ID NO:81)	(SEQ ID NO:82) FRGFSF	, ,
•	(SEQ ID NO:81) SFCGTIEYMAPE (SEQ ID NO:83)	(SEQ ID NO:82) FRGFSF (SEQ ID NO:84)	, ,
p90-RSK3	(SEQ ID NO:81) SFCGTIEYMAPE (SEQ ID NO:83)	(SEQ ID NO:82) FRGFSF (SEQ ID NO:84) FQGYSF	(CAA59427)
p90-RSK3	(SEQ ID NO:81) SFCGTIEYMAPE (SEQ ID NO:83) SFCGTIEYMAPD (SEQ ID NO:85)	(SEQ ID NO:82) FRGFSF (SEQ ID NO:84) FQGYSF (SEQ ID NO:86)	(CAA59427)
p90-RSK3 MSK1	(SEQ ID NO:81) SFCGTIEYMAPE (SEQ ID NO:83) SFCGTIEYMAPD (SEQ ID NO:85)	(SEQ ID NO:82) FRGFSF (SEQ ID NO:84) FQGYSF (SEQ ID NO:86) FQGYSF	(CAA59427) (AAC31171)
p90-RSK3 MSK1	(SEQ ID NO:81) SFCGTIEYMAPE (SEQ ID NO:83) SFCGTIEYMAPD (SEQ ID NO:85) SFCGTIEYMAPE (SEQ ID NO:87)	(SEQ ID NO:82) FRGFSF (SEQ ID NO:84) FQGYSF (SEQ ID NO:86) FQGYSF (SEQ ID NO:88)	(CAA59427) (AAC31171)

Table 2. Alignment of the amino acid sequences surrounding the T-loop and the hydrophobic motif of AGC kinases. All the sequences and accession numbers are from human proteins. The underlined residues correspond to those that become phosphorylated. Footnotes: (1) PDK1 does not possess a hydrophobic motif.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the

protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamavor et al (1999) Curr Biol 9, 186-197.

The PDK1 may also be a polypeptide with the amino acid sequence of residues 51 to 359 or 404 (or 71 to 360) of full-length human PDK1; this may comprise the protein kinase domain of PDK1, as described in Example 2. The PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may also be Myc epitope-tagged or His-tagged, as described in Example 1. The p70 S6 kinase, for example, may have a His tag at its N-terminus and/or may lack the carboxy terminal 104 residues (p70 S6K-T2). The PDK1 or SGK may be a *Saccharomyces cerevisiae* homologue, for example Pkh1 or Pkh2 (PDK1 homologues) or Ypk1 or Yrk2 (SGK homologues), as described in Casamayor et al (1999) Curr Biol 9, 186-197.

It is particularly preferred, although not essential, that the variant or fragment or derivative or fusion of the PDK1, or the fusion of the variant or fragment or derivative has at least 30% of the enzyme activity of full-length human PDK1 with respect to the phosphorylation of full-length human PKB α on residue Thr308 or SGK1 on residue Thr 256 in either the presence or absence of PtdIns(3,4,5)P $_3$ or PtdIns(3,4)P $_2$. It is more preferred if the variant or fragment or derivative or fusion of the said protein kinase, or the fusion of the variant or fragment or derivative has at least 50%, preferably at least 70% and more preferably at least 90% of the enzyme activity of

PDK1 with respect to the phosphorylation of PKBα or SGK1. However, it will be appreciated that variants or fusions or derivatives or fragments which are devoid of enzymatic activity may nevertheless be useful, for example by interacting with another polypeptide. Thus, variants or fusions or derivatives or fragments which are devoid of enzymatic activity may be useful in a binding assay, which may be used, for example, in a method of the invention in which modulation of an interaction of a mutated PDK1 of the invention and optionally also PDK1 with a interacting polypeptide or compound, for example an interacting polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr (SEQ ID NO:92), for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Zaa-Phe/Tyr (SEQ ID NO:93), for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Asp/Glu-Phe/Tyr (SEQ ID NO:94) or Phe/Tyr-Xaa-Xaa-Phe/Tyr-PhosphoSer/PhosphoThr-Phe/Tyr (SEQ ID NO:95) is measured.

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It is preferred that the variant or fragment or derivative or fusion of the said hydrophobic/phosphate binding pocket-containing protein kinase, or the fusion of the variant or fragment or derivative comprises a hydrophobic pocket and a phosphate binding pocket in the position equivalent to the hydrophobic and phosphate binding pocket of human PDK1, as discussed further below.

Equivalent preferences apply to a variant or fragment or derivative or fusion of the SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKC8, PKCζ or PRK2 (for example), or the fusion of the variant or fragment or derivative, with the substitution in relation to SGK, PKB and p70S6 kinase of the peptide substrate Crosstide (GRPRTSSFAEG, SEQ ID NO:96), or for PKB and SGK of the peptide substrate RPRAATF; the substitution in relation to PKA of the peptide substrate Kemptide (LRRASLG, SEQ ID NO:97); the substitution in relation to PKC isoforms and PRK1/2 of histone H1; and the

substitution in relation to MSK1/2 or p90-RSK1/2/3 of CREBtide (EILSRRPSYRK, SEQ ID NO:98).

By "variants" of a polypeptide we include insertions, deletions and substitutions, either conservative or non-conservative. In particular we include variants of the polypeptide where such changes do not substantially alter the activity of the said polypeptide, for example the protein kinase activity of PDK1, as described above.

By "conservative substitutions" is intended combinations such as Gly, Ala; Val, Ile, Leu; Asp, Glu; Asn, Gln; Ser, Thr; Lys, Arg; and Phe, Tyr.

The three-letter amino acid code of the IUPAC-IUB Biochemical Nomenclature Commission is used herein, with the exception of the symbol Zaa (negatively charged amino acid). In particular, Xaa represents any amino acid. It is preferred that Xaa and Zaa represent a naturally occuring amino acid. It is preferred that at least the amino acids corresponding to the consensus sequences defined above are L-amino acids.

It is particularly preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of PDK1 referred to above (or the sequence for SGK (including SGK1, 2 and 3), PKB, PKA or p70 S6 kinase, for example, as appropriate, referred to above), more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 85%, in still more preferably at least 85%, in further preference at least 85% or 97% identity with the amino acid sequence defined above.

It is still further preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase, as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of the catalytic domain, particularly the residues forming the hydrophobic pocket, of PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) in the appropriate sequence referred to above, more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 83 or 85%, in still further preference at least 80% and most preferably at least 95% or 97% identity with the amino acid sequence defined above. It will be appreciated that the catalytic domain of a protein kinase-related polypeptide may be readily identified by a person skilled in the art, for example using sequence comparisons as described below.

The percent sequence identity between two polypeptides may be determined using suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group and it will be appreciated that percent identity is calculated in relation to polypeptides whose sequence has been aligned optimally.

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The alignment may alternatively be carried out using the Clustal W program (Thompson *et al* (1994) *Nucl Acid Res* **22**, 4673-4680). The parameters used may be as follows:

Fast pairwise alignment parameters: K-tuple(word) size; 1, window size; 5, gap penalty; 3, number of top diagonals; 5. Scoring method: x percent.

Multiple alignment parameters: gap open penalty; 10, gap extension penalty; 0.05.

Scoring matrix: BLOSUM.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor et al (1999) Curr Biol 9, 186-197.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide that is capable of interacting with a polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr (SEQ ID NO:92), preferably Phe-Xaa-Xaa-Phe/Tyr, more preferably Phe-Xaa-Xaa-Phe, still more preferably Phe/Tyr-Xaa-Xaa-Phe/Tyr-Xaa-Phe/Tyr (SEQ ID NO:93) or Phe/Tyr-Xaa-Xaa-Phe/Tyr-COOH, for example the polypeptide PIF or PIFtide, as defined below. Further preferences for the said polypeptide are as given above.

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The protein kinase activity of PKB, SGK or p70 S6 kinase that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Arg-Xaa-Arg-Xaa-Xaa-Ser/Thr (SEQ_ID_NO:100). The polypeptide may be Glycogen Synthase Kinase 3 (GSK3), 40 S ribosomal subunit S6, BAD, 6-phosphofructo-2-kinase, phosphodiesterase3b, human caspase 9, endothelial nitric oxide synthase or BRCA1.

A compound identified by a method of the invention may modulate the ability of the protein kinase to phosphorylate different substrates, for example different naturally occuring polypeptides, to different extents. The compound may inhibit the protein kinase activity in relation to one substrate but may increase the protein kinase activity in relation to a second substrate. For example, the protein kinase activity of PDK1 may be modulated to a different extent for PKB when compared with SGK, p70 S6 kinase and/or PKC

It will be appreciated that the modulatory, for example inhibitory action of a compound found to bind (or inhibit binding of a polypeptide or compound) to the protein kinase may be confirmed by performing an assay of enzymic activity (for example PDK1 and/or PDK2 protein kinase activity) in the presence of the compound.

By "hydrophobic pocket-containing protein kinase having a hydrophobic pocket (PIF binding pocket) in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150," is meant a polypeptide having an amino acid sequence identifiable as that of a protein kinase catalytic domain, and further having a predicted or determined three-dimensional structure that includes a hydrophobic pocket corresponding to the region indicated in Example 1 as the PIF binding pocket, and a pocket corresponding to the region indicated in Example 1 as the phosphate binding pocket. The hydrophobic pocket and phosphate binding pockets in PDK1 do not overlap with the ATP or phosphorylation site binding sites on PDK1

It is preferred that the protein kinase has identical or conserved residues that are equivalent to Lys 115, Ile118, Ile119, Val124, Val127 and/or Leu 155 of human PDK1, more preferably at least Lys115 and Leu155 of human PDK1, most preferably an identical residue equivalent to Leu155. Thus, for example, the protein kinase may have a Lys residue at the position equivalent to Lys115 of PDK1 and/or a Leu residue at the position equivalent to Leu155 of PDK1. It is preferred that the protein kinase does not have an Ala at the position equivalent to Lys115 and/or a Ser, Asp or Glu at the position equivalent to Leu155 of PDK1.

It is further preferred that the protein kinase has identical or conserved residues that are equivalent to Lys76, Arg131, Thr148 and/or Gln 150 of human PDK1, more preferably at least Lys76 and Gln150 of human PDK1, most preferably an identical residue equivalent to Gln150. Figure 5B shows an alignment of examples of protein kinases considered to have a phosphate binding pocket at the position equivalent to the said phosphate binding pocket of PDK1. Sequence conservation/preferred residues at the positions identified are discussed further in Example 1.

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An amino acid sequence may be identifiable as that of a protein kinase catalytic domain by reference to sequence identity or similarities of three dimensional structure with known protein kinase domains, as known to those skilled in the art.

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Protein kinases show a conserved catalytic core, as reviewed in Johnson et al (1996) Cell, 85, 149-158 and Taylor & Radzio-Andzelm (1994) Structure 2, 345-355. This core folds into a small N-terminal lobe largely comprising anti-parallel β-sheet, and a large C-terminal lobe which is mostly α-helical.

A deep cleft at the interface between these lobes is the site of ATP binding, with the phosphate groups near the opening of the cleft.

Protein kinases also show conserved sequences within this catalytic core, and the residue equivalent to a given residue of, for example, PDK1, may be identified by alignment of the sequence of the kinase with that of known kinases in such a way as to maximise the match between the sequences. The alignment may be carried out by visual inspection and/or by the use of suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group, which will also allow the percent identity of the polypeptides to be calculated. The Align program (Pearson (1994) in: Methods in Molecular Biology, Computer Analysis of Sequence Data, Part II (Griffin, AM and Griffin, HG eds) pp 365-389, Humana Press, Clifton).

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The comparison of amino acid sequences or three dimension structure (for example from crystallography or computer modelling based on a known structure) may be carried out using methods well known to the skilled man, for example as described in WO 01/44497.

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MAP kinase, MEK1, Cdk2 and Erk2 (for example) are not protein kinases having a hydrophobic pocket in the position equivalent to the hydrophobic (PIF binding) pocket of PDK1. MEK1, Cdk2 and ERK2 may have a larger hydrophobic pocket which interacts with an amino acid sequence motif (which may be Phe-Xaa-Phe-Pro, SEQ ID NO:101) which is not Phe-Xaa-Xaa-Phe (SEQ ID NO:99). Thus, these protein kinases do not have a hydrophobic pocket in the position equivalent to the said hydrophobic (PIF-binding) pocket of PDK1.

A further aspect of the invention provides a mutated protein kinase, wherein the protein kinase before mutation has a hydrophobic pocket in the position equivalent to the hydrophobic pocket (PIF-binding pocket) of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further has a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, and wherein one or more residues equivalent to Ile118, Val124, Val127, Lys76 or Thr148 forming part of the hydrophobic pocket or phosphate binding pocket of the protein kinase is mutated. It is preferred that the said protein kinase is PDK1. The said protein kinase may alternatively be, for example, SGK, PKB or p70 S6 kinase. It is particularly preferred that the residue at the position equivalent to residue Lys76 of PDK1 is mutated to an Ala. The mutated protein kinase may be useful in determining whether a polypeptide or compound interacts with the hydrophobic (PIF binding) pocket or phosphate binding pocket of the unmutated protein kinase. For example, the abilities of a compound (including polypeptide) to bind to the mutated and unmutated protein kinase, or to modulate the activity of the protein kinase towards one or more substrates of the protein kinase, may be measured and compared.

The mutated protein kinase may alternatively or in addition be mutated at a residue forming part of the "hydroxyl-pocket" discussed in Example 6, for example the residue equivalent to Thr222 and/or Gln 220 of full length human PDK1. These residues are involved in the binding of the UCN-01 7-hydroxyl group.

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A further aspect of the invention provides a polynucleotide encoding a mutated protein kinase of the invention. A still further aspect of the invention provides a recombinant polynucleotide suitable for expressing a

mutated protein kinase of the invention. A yet further aspect of the invention provides a host cell comprising a polynucleotide of the invention.

A further aspect of the invention provides a method of making a mutated protein kinase of the invention, the method comprising culturing a host cell of the invention which expresses said mutated protein kinase and isolating said mutated protein kinase.

A further aspect of the invention provides a mutated protein kinase obtainable by the above method.

Examples of these aspects of the invention are provided in Example 1, and may be prepared using routine methods by those skilled in the art, for example as described in WO 00/35946.

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For example, the above mutated protein kinase may be made by methods well known in the art and as described below and in Example 1 or 2, for example using molecular biology methods or automated chemical peptide synthesis methods.

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It will be appreciated that peptidomimetic compounds may also be useful. Thus, by "polypeptide" or "peptide" we include not only molecules in which amino acid residues are joined by peptide (-CO-NH-) linkages but also molecules in which the peptide bond is reversed. Such retro-inverso peptidomimetics may be made using methods known in the art, for example such as those described in Mézière et al (1997) J. Immunol. 159, 3230-3237, incorporated herein by reference. This approach involves making pseudopeptides containing changes involving the backbone, and not the orientation of side chains. Retro-inverse peptides, which contain NH-CO

bonds instead of CO-NH peptide bonds, are much more resistant to proteolysis.

Similarly, the peptide bond may be dispensed with altogether provided that an appropriate linker moiety which retains the spacing between the $C\alpha$ atoms of the amino acid residues is used; it is particularly preferred if the linker moiety has substantially the same charge distribution and substantially the same planarity as a peptide bond.

It will be appreciated that the peptide may conveniently be blocked at its Nor C-terminus so as to help reduce susceptibility to exoproteolytic digestion.

The invention further provides a method of identifying a compound that modulates the protein kinase activity of a protein kinase having a hydrophobic pocket and phosphate binding pocket in the positions equivalent to the hydrophobic (PIF binding) pocket and phosphate binding pocket of PDK1, as defined above (for example PDK1), comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to the said mutated protein kinase of the invention.

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The method may further comprise determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to, the protein kinase (for example PDK1) which is not mutated at the said residue. When the protein kinase is PDK1, it may lack a functional PH domain (ie it may lack a PH domain capable of binding a phosphoinositide).

It will be appreciated that the protein kinase or mutated protein kinase may be a fusion protein comprising a tag, for example to aid purification, for example a GST tag, as described in Example 1. The capability of the said PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) polypeptide with regard to interacting with or binding to a polypeptide or other compound may be measured by any method of detecting/measuring a protein/protein interaction or other compound/protein interaction, as discussed further below. Suitable methods include methods analagous to those described in Example 1, as well as other methods, for example yeast two-hybrid interactions, co-purification, ELISA, co-immunoprecipitation and surface plasmon resonance methods. Thus, the said PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may be considered capable of binding to or interacting with a polypeptide or other compound if an interaction may be detected between the said PDK1 polypeptide and the said interacting polypeptide by ELISA, co-immunoprecipitation or surface plasmon resonance methods or by a yeast two-hybrid interaction or copurification method, for example as described in Example 1.

It is preferred that the interaction can be detected using a surface plasmon resonance method, as described in Example 1. The interacting polypeptide (for example a polypeptide comprising a phosphorylated "hydrophobic motif", for example S6K-pHM; see example 1) may be immobilised on the test surface, for example it can be coupled through amino groups to a SensorChip CM5TM, according to the manufacturer's instructions, or a biotinylated polypeptide can be bound to an avidin coated SensorChip SA. The protein kinase (at concentrations between, for example 0 and between $10\mu M$ and $1.0\mu M$, for example $2\mu M$) is then injected over the surface and steady state binding determined in each case. From these measurements a K_d can be determined. It is preferred that the interaction has a K_d of less than $8\mu M$, more preferably less than $5\mu M$, $2\mu M$, $1\mu M$, 500n M, 300n M, 200n M or 100n M, for example about 150n M. Alternatively, a K_d can be determined for a polypeptide or other compound in competition with the immobilised polypeptide (or other compound). The protein kinase (for

example at a concentration of 0.5 µM) is mixed with free polypeptide (for example, at concentrations between 0 and 3uM) and the mixture injected over the immobilised polypeptides. The steady state binding is determined in each case, from which the K_d of the interaction can be determined using the Cheng-Prescott relationship. Alternatively, the interaction may be expressed in terms of an observed response or relative observed responses, measured in terms of mass of protein bound to the surface, as described in Example 2. For example, the polypeptide may be immobilised by amino coupling to a SensorChip CM5 and each protein kinase (for example different mutated protein kinases, as discussed below) for example at a concentration of 1.0µM or a range of concentrations, injected over the immobilised polypeptide. Alternatively, the polypeptide may be immobilised on a SA SensorChip and each protein kinase, for example at a concentration of 40nM or a range of concentrations injected over the immobilised polypeptide. The steady state response for each protein kinase is determined, for example expressed in Response Units (RU), 1000RU corresponds to 1 ng/mm2 of protein bound to the surface. A response of less than 10RU may indicate that no interaction has taken place. A response of at least 10RU may indicate that the immobilised and injected molecules interact with each other.

It will be appreciated that the above methods may be used to determine whether a particular polypeptide or compound interacts with a protein kinase or mutated protein kinase.

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The effect of the compound on the rate or degree of phosphorylation of a hydrophobic pocket and/or phosphate binding pocket-dependent substrate may be determined. A compound may be selected that decreases the protein kinase activity of the said protein kinase, for example PDK1,

towards a hydrophobic pocket-dependent substrate or a phosphate binding pocket-dependent substrate and does not affect or increases the protein kinase activity towards a hydrophobic pocket or phosphate binding pocket-independent substrate, for example PKB when the kinase is PDK1. An activator of PDK1 may mimic insulin and may be useful in treating diabetes or obesity, and may protect cells from apoptosis.

Compounds that bind specifically to the phosphate binding site may activate PDK1 (or other AGK kinase having a phosphate binding site). Also compounds that bind to the residues forming part of the pohsphate binding site might transduce the negative effect and inhibit the kinase activity. A compound interacting with the phosphate binding site of PDK1 may be an activator, but only of a subset of substrates. Some substrates of PDK1 require the interaction with the phosphate binding site, such as S6K and SGK.

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To generate a specific molecule that could bind to the phosphate and/or PIF-binding pocket of PDK1 a anti-idiotype strategy using combinatorial RNA libraries could be employed. Previous studies have established that Combinatorial RNA libraries can be used to isolate specific ligands, called aptamers, for virtually any target molecule by a procedure probably best known as SELEX (Ellington, A. D., and Szostak, J. W. (1990) Nature 346, 818-822; Tuerk, C., and Gold, L. (1990) Science 249, 505-510). Using this approach RNA molecules that interact with antibodies raised against PIFtide or peptides that encompass the hydrophobic motif of AGC kinases which are phosphorylated at their hydrophobic motif would be selected (preferably antibodies that are specific for the phosphorylated form ie bind the phosphorylated form but not the non-phosphorylated form). These RNA species then may have the intrinsic conformation to interact with the phosphate binding (and possibly also the PIF-binding) pocket(s) of PDK1.

Antibodies to the phosphate binding pocket may be produced. For example, animals could be immunised with wild type PDK1. Serum could then be purified with a column where the resin is coated with wild type PDK1 used for the immunisation. Specific antibodies could then be passed through columns coated with mutant PDK1 molecules differing only in that they have specific mutations in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala. Antibodies that don't bind to this mutant will either be specific antibodies that recognise the specific motifs or antibodies that are sensitive to the conformational changes associated with these mutations. The opposite development could also be performed: antibodies against a mutant PDK1 having a specific mutation(s) in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala, could be produced and the serum further purified through columns coated with wild type PDK1.

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Thus, a further aspect of the invention provides an antibody reactive with the phosphate binding pocket of PDK1 or other hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150. A further aspect of the invention provides an antibody reactive with PDK1 or other phosphate-binding pocket—containing protein kinase as defined above but not with the said protein kinase mutated at the phosphate binding site, or vice versa. A further aspect of the invention provides a method for preparing or selecting an antibody wherein the antibody is prepared or selected against a said protein kinase (for example

PDK1) unmutated at the phosphate binding site and a said protein kinase mutated at the phosphate binding site.

By the term "antibody" is included synthetic antibodies and fragments and variants (for example as discussed above) of whole antibodies which retain the antigen binding site. The antibody may be a monoclonal antibody, but may also be a polyclonal antibody preparation, a part or parts thereof (for example an F_{ab} fragment or $F(ab')_2$) or a synthetic antibody or part thereof. Fab, Fv, ScFv and dAb antibody fragments can all be expressed in and secreted from E. coli, thus allowing the facile production of large amounts of the said fragments. By "ScFv molecules" is meant molecules wherein the V_H and V_L partner domains are linked via a flexible oligopeptide. IgG class antibodies are preferred.

Suitable monoclonal antibodies to selected antigens may be prepared by known techniques, for example those disclosed in "Monoclonal Antibodies: A manual of techniques", H. Zola (CRC Press, 1988) and in "Monoclonal Hybridoma Antibodies: techniques and Applications", JGR Hurrell (CRC Press, 1982), modified as indicated above. Bispecific antibodies may be prepared by cell fusion, by reassociation of monovalent fragments or by chemical cross-linking of whole antibodies. Methods for preparing bispecific antibodies are disclosed in Corvalen et al, (1987) Cancer Immunol. Immunother. 24, 127-132 and 133-137 and 138-143.

25 A general review of the techniques involved in the synthesis of antibody fragments which retain their specific binding sites is to be found in Winter & Milstein (1991) Nature 349, 293-299.

For example, an antibody that does not bind PDK1 Arg131Ala could be specifically recognising this residue in the phosphate binding site, but could

also be recognising specifically the inactive conformation of PDK1, which is stabilised by Arg 131. The opposite development could also be performed: antibodies against a mutant PDK1 Arg131Ala could be produced and the serum further purified through columns coated with wild type PDK1. In this way, antibodies may be prepared that would either not be able to interact with the phosphate binding site Arg 131 but only when a small residue is in its place, or antibodies that are probes for the active conformation of PDK1. These conformational probes could be used in high throughoutput screenings, HTS, in the search of compounds that are capable of modifying the conformation of the given protein kinase. Antibodies could have been produced with previous knowledge to detect active protein kinases by immunising with active protein kinases, but in those cases, the antibodies would have recognised also the phosphorylation events that make a protein kinase be active. In the methodology here described using antibodies, the conformational probes could be easily isolated. Furthermore, antibodies obtained from an active protein kinase (with overall modifications that make it active) could be further purified through a column coated with the inactive protein kinase (keeping the non bound fraction) and then further purifyied on a column coated with a protein kinase consisting of an activating mutation (such as R131A in the case of PDK1), retaining the specifically bound fraction, which could be an active conformation probe. This type of approach could also allow the development of conformation specific probes by the use of activating or inhibiting mutations.

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A further aspect of the invention provides a kit of parts useful in carrying out a method according to the preceding aspect of the invention, comprising (1) a mutated protein kinase of the invention and (2) the protein kinase which is not a mutated said protein kinase as defined above.

The protein structures described herein (for example with the co-ordinates shown in Examples 2, 3 or 4, or structures modelled thereon) may be useful in designing further reagents that may be useful in drug screening assays or characterisation of protein kinase activity or regulation. For example, such structures may be useful in designing mutants that may be useful in FRETbased activities, for example in which surface residues near to binding sites are mutated to cysteines to allow coupling of chromophores. For example, the cysteine residue may be fluorescently-labelled, and a change in fluorescence intensity or frequency may be detected in an assay. Any thiolreactive fluorophore, for example BADAN (see, for example, Wadum et al Fluorescently labeled bovine acyl-CoA binding protein - an acyl-CoA sensor. Interaction with CoA and acvl-CoA esters and its use in measuring free acyl CoA esters and non-esterified fatty acids (NEFA): Hammarstrom et al (2001) Biophys J 80(6), 2867-2885; Schindel et al (2001) Eur J Biochem 268(3), 800-808), could be used to label the cysteine. An alternative suitable fluorophore is Acrylodan (Richieri et al (1992) J Biol Chem 267(33), 23495-23501).

20 It will be appreciated that the invention provides screening assays for drugs which may be useful in modulating, for example either enhancing or inhibiting, the protein kinase activity of a protein kinase (for example, the protein kinase activity towards a particular substrate) having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of Protein Kinase A (PKA) that is defined by residues including Lys76, Leu116, Val80 and/or Lys111 of full-length mouse PKA, for example PDK1, SGK, PKB, PKA or p70 S6 kinase, for example the PDK1 or PDK2 activity (as discussed above) of PDK1. The compounds identified in the methods may

themselves be useful as a drug or they may represent lead compounds for the design and synthesis of more efficacious compounds.

The compound may be a drug-like compound or lead compound for the development of a drug-like compound for each of the above methods of identifying a compound. It will be appreciated that the said methods may be useful as screening assays in the development of pharmaceutical compounds or drugs, as well known to those skilled in the art.

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The term "drug-like compound" is well known to those skilled in the art, and may include the meaning of a compound that has characteristics that may make it suitable for use in medicine, for example as the active ingredient in a medicament. Thus, for example, a drug-like compound may be a molecule that may be synthesised by the techniques of organic chemistry, less preferably by techniques of molecular biology or biochemistry, and is preferably a small molecule, which may be of less than 5000 daltons. A drug-like compound may additionally exhibit features of selective interaction with a particular protein or proteins and be bioavailable and/or able to penetrate cellular membranes, but it will be appreciated that these features are not essential.

The term "lead compound" is similarly well known to those skilled in the art, and may include the meaning that the compound, whilst not itself suitable for use as a drug (for example because it is only weakly potent against its intended target, non-selective in its action, unstable, difficult to synthesise or has poor bioavailability) may provide a starting-point for the design of other compounds that may have more desirable characteristics.

It is appreciated that screening assays which are capable of high throughput

operation are particularly preferred. Examples may include cell based

assays and protein-protein binding assays. An SPA-based (Scintillation Proximity Assay; Amersham International) system may be used. For example, beads comprising scintillant and a substrate polypeptide or interacting polypeptide may be prepared. The beads may be mixed with a sample comprising ³²P- or ³³P-γ-labelled PDK1 or other protein kinase or mutated protein kinase (as defined above) and with the test compound. Conveniently this is done in a 96-well or 384-well format. The plate is then counted using a suitable scintillation counter, using known parameters for ³²P or ³³P SPA assays. Only ³²P or ³³P that is in proximity to the scintillant, i.e. only that bound to the substrate or interacting polypeptide that is bound to the beads, is detected. Variants of such an assay, for example in which the substrate or interacting polypeptide is immobilised on the scintillant beads *via* binding to an antibody or antibody fragment, may also be used.

It will be understood that it will be desirable to identify compounds that may modulate the activity of the protein kinase *in vivo*. Thus it will be understood that reagents and conditions used in the method may be chosen such that the interactions between, for example, the said protein kinase and the interacting polypeptide, are substantially the same as between the human protein kinase and a naturally occurring interacting polypeptide comprising the said amino acid sequence. It will be appreciated that the compound may bind to the protein kinase, or may bind to the interacting polypeptide.

The compounds that are tested in the screening methods of the assay or in other assays in which the ability of a compound to modulate the protein kinase activity of a protein kinase, for example a hydrophobic pocket-containing protein kinase, as defined above, may be measured, may be compounds that have been selected and/or designed (including modified)

using molecular modelling techniques, for example using computer techniques.

A further aspect of the invention is a compound identified or identifiable by the above selection/design methods of the invention, for example an RNA molecule or antibody identifiable as defined above.

A still further aspect of the invention is a compound (or polypeptide or polynucleotide) of the invention or identified or identifiable by the above selection/design methods of the invention, for use in medicine. Conditions or diseases in which such compounds, polypeptides or polynucleotides may be useful are indicated below.

The compound (or polypeptide or polynucleotide) may be administered in any suitable way, usually parenterally, for example intravenously, intraperitoneally or intravesically, in standard sterile, non-pyrogenic formulations of diluents and carriers. The compound (or polypeptide or polynucleotide) may also be administered topically, which may be of particular benefit for treatment of surface wounds. The compound (or polypeptide or polynucleotide) may also be administered in a localised manner, for example by injection. The compound may be useful as an antifungal (or other parasitic, pathogenic or potentially parasitic or pathogenic organism) agent.

A further aspect of the invention is the use of a compound (or polypeptide or polynucleotide) as defined above in the manufacture of a medicament for the treatment of a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket, as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6

kinase/PRK2/PKC signalling. The patient may be in need of inhibition of a said hydrophobic/phosphate binding pocket-containing kinase in an infecting organism, for example the patient may have a fungal infection for which treatment is required. The compound may inhibit the infecting organism's (for example fungal) hydrophobic/phosphate binding pocket-containing protein kinase, but may not inhibit the patient's equivalent hydrophobic/phosphate binding pocket-containing protein kinase.

A further aspect of the invention is a method of treating a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling, wherein the patient is administered an effective amount of a compound (or polypoptide or polynucleotide) as defined above.

A compound that is capable of reducing the activity of PKC, for example PKCβ, PRK1 or 2, PDK1 (ie the PDK1 and/or the PDK2 activity), PKB, SGK or p70 S6 kinase may be useful in treating cancer. PDK1, for example via PKB and/or SGK, may be capable of providing a survival signal that protects cells from apoptosis induced in a variety of ways (reviewed in Cross et al (1995) Nature 378, 785-789 and Alessi & Cohen (1998) Curr. Opin. Genetics. Develop. 8, 55-62). Thus, such compounds may aid apoptosis. Reduction of the activity of PDK1, PKB, SGK and/or p70 S6 kinase may promote apoptosis and may therefore be useful in treating cancer. Conditions in which aiding apoptosis may be of benefit may also include resolution of inflammation.

A compound is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase may be useful in treating diabetes or obesity, or may be useful in inhibiting apoptosis. Increased activity of PDK1, PKB, SGK or p70 S6 kinase may lead to increased levels of leptin, as discussed above, which may lead to weight loss; thus such compounds may lead to weight loss. For example, such compounds may suppress apoptosis, which may aid cell survival during or following cell damaging processes. It is believed that such compounds are useful in treating disease in which apoptosis is involved. Examples of such diseases include, but are not limited to, mechanical (including heat) tissue injury or ischaemic disease, for example stroke and myocardial infarction, neural injury and myocardial infarction. Thus the patient in need of modulation of the activity of PDK1, PKB, SGK or p70 S6 kinase may be a patient with cancer or with diabetes, or a patient in need of inhibition of apoptosis, for example a patient suffering from tissue injury or ischaemic injury, including stroke.

Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identified or identifiable by the screening methods of the invention.

20 A still further invention provides a use of a compound identifiable by the screening methods of the invention in the manufacture of a medicament for treating an ischaemic disease in a patient.

Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identifiable by the screening methods of the invention

If the patient is a patient in need of promotion of apoptosis, for example a
patient with cancer, it is preferred that the compound of the invention that is

used in the preparation of the medicament is capable of reducing the activity of PDK1, PKB, SGK or p70 S6 kinase. If the patient is a patient with diabetes or a patient in need of inhibition of apoptosis, for example a patient with ischaemic disease, it is preferred that the compound of the invention that is used in the preparation of the medicament is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase.

All documents referred to herein are hereby incorporated by reference.

10 The invention is now described in more detail by reference to the following, non-limiting, Figures and Examples.

Figure legends

1. Overview of the PDK1 structure.

The PDK1 kinase domain backbone is shown in a ribbon representation, with the secondary structure elements for residues 74-163 in the lower half of the Figure and for residues 164- 358 in the upper part of the Figure. Helix αG, encompassing residues 287-295 (which makes a crystal contact to a symmetry related PDK1 molecule, Fig. 2), is at the bottom right of the Figure. Key residues discussed in the text are shown as a sticks model. ATP is shown as a sticks model. A simulated annealing [Fo –[Fc', φ calc map is shown in black, contoured at 3 σ. The phosphoserine and the sulphate discussed in the text are also shown.

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2. The PIF-pocket

A. A surface representation of the putative PIF binding pocket is shown and compared to the pocket interacting with the C-terminal FXXF (SEQ ID NO: 1) motif in PKA. For PDK1, the αG helix of a symmetry-related molecule

is shown as a ribbon, in PKA the C-terminus is also shown as a ribbon. Aromatic amino acids buried in the pocket are shown as sticks; further side chains interacting with the pocket are also shown as sticks. Helix α C is also shown as a ribbon in both PDK1 and PKA (at bottom of images). In PDK1, the ordered sulphate ion and basic residues interacting with it are also shown

B. A stereo image of the residues lining the PIF-pocket is shown. The PDK1 backbone is shown as a grey ribbon. Side chains are shown as sticks. Hydrogen bonds to the sulphate ion are shown as black dotted lines.

3. Structure-based sequence alignment

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The sequences of PKA (SEQ ID NO: 103) and PDK1 (SEQ ID NO:102) are aligned according to a structural superposition performed in WHAT IF [Vriend, 1990]. Sequence numbering is according to PDK1. β -strands (arrows) and α -helices (bars) are shown for the PDK1 structure according to a DSSP [Kabsch and Sander, 1983] secondary structure assignment, and labelled consistent with the secondary structure element names proposed for PKA [Taylor and Radzioandzelm, 1994]. Residues lining the PIF-pocket are indicated with a black dot. Residues hydrogen bonding the sulphate ion are indicated by arrows. The PDK1 residues equivalent to Ser53 and Gly186 in PKA, are labelled with an asterisk.

4. PDK1 binding & activation studies

Binding and activation of wild type and mutant forms of PDK1 to a phosphopeptide derived from the hydrophobic motif of S6K1. The binding of the wild type (wt) PDK1 and indicated mutants to a phosphopeptide comprising the hydrophobic motif of S6K1 (S6K-pHM: SESANQVFLGFT*YVAPSV, where T* indicates phospho-threonine, SEQ

ID NO:104) was analysed by surface plasmon resonance as described in the Materials and Methods

A. The sensor chip SA was coated with 12RUs of the biotinylated S6K-pHM peptide and the binding was analysed following injection of 270 nM wild type PDK1, PDK1 [T148A] and PDK1 [K76A]. No detectable binding to S6K-pHM was observed using PDK1 [R131A] or PDK1 [Q150] (data not shown).

B. As in A. except that binding was analysed over a range of PDK1 concentrations (2-2150nM). The response level at the steady state binding is plotted versus the log of the PDK1 concentration. The estimated Kd was obtained by fitting the data to a sigmoid curve using Kaleidagraph software. Kd for wild type PDK1 was 642 – 131 nM, PDK1 [T148A] was 64 – 7 nM and PDK1 [K76A] was 1744 – 167 nM. No detectable binding of PDK1 to the non-phosphorylated S6K-HM peptide (SESANQVFLGFTYVAPSV, SEQ ID NO:105) was detected with wild type PDK1or any of the mutants (data not shown).

C. Activation of the indicated forms of PDK1 by S6K-pHM and S6K-HM.
PDK1 activity was measured using the peptide substrate (T308tide) in the presence of the indicated concentrations of S6K-pHM (closed circles) and S6K-HM (open circles) as described in the methods. Assays were performed in triplicate and similar results obtained in 2 separate experiments. The results are the average – SD for a single experiment.

25 5. Interactions of regulatory phosphates with the αC helix

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A. The PDK1 backbone is shown as a ribbon, with helix α C in the centre of the view. Key residues are shown as sticks. The sulphate ion and the phosphate on the activation loop are also shown. A sticks model of ATP is shown. Hydrogen bonds are shown as black dotted lines.

B. Alignment of the amino acid sequence forming part of the phosphate pocket on PDK1 with the equivalent region of the indicated AGC kinases. Identical residues are denoted by white letters on a black background and similar residues by gray boxes. Arrows indicate the residues corresponding to Lys 76, Arg131, Thr148 and Gln150 of PDK1 (SEQ ID NOs:12 and 144). The aligned amino acid sequences are as follows: PKBα (SEQ ID NOs: 13 and 145), S6K1 (SEQ ID NOs: 14 and 146), SGK1 (SEQ ID NOs: 15 and 147), and Rsk1 (SEO ID NOs: 16 and 148).

6. Essential dynamics

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A. Projection of all available PKA crystal structures (labelled dots) and the PDK1 structure (diamond) onto the first two eigenvectors (i.e. the ones with the two largest eigenvalues) calculated from the PKA structures.

B. Graphic representation of the motion along the first eigenvector, generated by projecting two structures at -4 nm (black) and +4 nm (grey).

7. Alignment of AGC protein kinase family members.

The alligned amino acid sequences and their respective corresponding sequence identifier are as follows:

P70S6Kalpha (SEQ ID NO: 17), P70S6Kbeta (SEQ ID NO: 18), P90RSK1 (SEQ ID NO: 19), P90RSK2 (SEQ ID NO: 20), P90RSK3 (SEQ ID NO: 21), MSK1 (SEQ ID NO: 22), MSK2 (SEQ ID NO: 23), PKBalpha (SEQ ID NO: 24), PKBbeta (SEQ ID NO: 25), PKBgamma (SEQ ID NO: 26), PRK1 (SEQ ID NO: 27), PRK2 (SEQ ID NO: 28), SGK1 (SEQ ID NO: 29), SGK3 (SEQ ID NO: 30), SGK2 (SEQ ID NO: 31), PKCbeta (SEQ ID NO: 32), PKCbetaII (SEQ ID NO: 33), PKCalpha (SEQ ID NO: 34), PKCgamma (SEQ ID NO: 35), PKCzeta (SEQ ID NO: 36), PKCiota (SEQ ID NO: 37), PKCdelta (SEQ ID NO: 38), PKAgamma (SEQ ID NO: 39), and PDK1 (SEQ ID NO: 40).

8. Staurosporine and UCN-01 electron density.

The staurosporine and UCN-01 molecules are shown in a stick representation. Hydrogen bonding atoms (Table 4) are labelled according to [49]. The unbiased $|F_o|$ - $|F_c|$, ϕ_{calc} maps are contoured at 2.5 σ .

9..Details of the inhibitor binding sites.

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The bridging water molecule is shown as a sphere. Hydrogen bonds are indicated by black dotted lines. Labelled residues hydrogen-bond the inhibitor molecules.

Example 1: High resolution crystal structure of the human PDK1 catalytic domain defines the regulatory phosphopeptide docking site

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) plays a key role in insulin/growth factor induced signalling pathways through phosphorylation of downstream AGC-kinases such as Protein Kinase B/Akt and p70 ribosomal S6 kinase (S6K1). Here we describe the 2.0 Å crystal structure of the PDK1 kinase domain in complex with ATP. The structure defines the hydrophobic pocket termed the 'PIF-pocket' which plays a key role in mediating the interaction and phosphorylation of certain substrates such as S6K1. In the PDK1 structure, this pocket is occupied by an extensive crystallographic contact with another molecule of PDK1, reminiscent of the interaction of Protein Kinase A with the hydrophobic motif at its C-terminus. Previous studies have shown that phosphorylation of S6K1 at its C-terminal PIF-pocket-interacting motif, promotes the binding of S6K1 with PDK1, suggesting that there may be a phosphate docking site located nearby the PIF-pocket. Interestingly, close to the PIFpocket on the PDK1 structure, there is an ordered sulphate ion, interacting tightly with four surrounding side chains. The roles of these residues were investigated through a combination of site directed mutagenesis and kinetic studies, the results of which suggest that this region of PDK1 does indeed represent a phosphate dependent docking site. An analogous phosphate binding regulatory motif may participate in the activation of other AGC kinases.

Results & Discussion

5 Overall structure

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The structure of the catalytic domain of PDK1 was solved by molecular replacement and refined to an R-factor of 0.19 (Rfree=0.22). PDK1 assumes the classic bilobal kinase fold (Fig. 1) and is similar to the only other AGC kinase structure solved, that of PKA (RMSD of 1.0 Å on C α atoms with PDB entry 1STC [Prade et al., 1997]). The form of PDK1 that was crystallized comprised residues 51 to 359. The tip of the activation loop (residues 233-236) is disordered, as observed in other kinase structures [Johnson et al., 1996]. The N-terminus (residue 51-70), which is pointing into a large void generated by the crystallographic symmetry, is also disordered. In contrast, the N-terminal extension to the kinase domain of PKA assumes an amphipathic a -helix (termed αA-helix), and packs against the kinase core [Knighton et al., 1991]. The cluster of hydrophobic residues that mediates this interaction in PKA is not present in PDK1, suggesting that the N-terminus of PDK1 could have a different function from that of PKA. Interestingly, it has recently been shown that the N-terminus of PDK1 (residues 1-50) interacts with Ral guanine nucleotide exchange factors [Tian et al., 2002]. Thus, this region may assume a unique conformation in PDK1. which is not defined by the structure described here.

25 PDK1 was crystallised in the presence of ATP but in the absence of any divalent cations. In the early stages of the refinement well-defined density for the entire ATP molecule could be observed. ATP adopts a different conformation to that observed in other kinase-ATP complexes (Fig. 1). Perhaps due to the absence of divalent cations, the generally observed kink between the β and γ phosphate caused by the interaction with such an ion, is not seen in the PDK1 structure.

s It is known that PDK1 can phosphorylate itself on residue Ser 241 in the activation loop and that this phosphorylation is required for PDK1 activity [Alessi et al., 1997]. Indeed, we observed density for a phosphate attached to this residue (Fig. 1), and extensive interactions are observed between this phosphoserine and residues from the C-terminal lobe and αC-helix (Fig. 1).

The interaction between Ser241 and the C-terminal lobe is similar to the equivalent interactions in PKA but as discussed below the binding to the αC-helix differs.

The PIF-pocket

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As outlined in the introduction, PDK1 was postulated to possess a pocket (the 'PIF-pocket') in the small lobe of its catalytic domain, required for the binding of PDK1 to the hydrophobic motif of its substrates [Biondi et al., 2000]. The PDK1 structure described here indeed reveals such a pocket, and shows that it lies in a location similar to the FXXF (SEQ ID NO:1)-binding pocket in PKA (Fig. 2). PDK1 residues Lys115, Ile118, Ile119 on the αB helix (Fig. 2), Val124, Val127 on the αC helix and Leu155 on β -sheet 5 form an approximately 5 Å deep pocket. Previous work has shown that mutation of Leu 155 to Glu abolishes the ability of PDK1 to interact with a peptide that encompasses the hydrophobic motif of PRK2 (PIFtide) [Biondi et al., 2000] as well as with S6K1, SGK1, PKC ζ and PRK2 [Balendran et al., 2000, Biondi et al., 2000]. In addition, mutation of Lys115, Ile119, Glu150, and Leu155 to alanine, reduced the affinity of PDK1 for PIFtide approximately 10-fold, but did not affect the ability to phosphorylate and

activate S6K1 and SGK1 [Biondi et al., 2001]. These results are in agreement with the crystal structure of the PIF-pocket, since Leu155 is located at the center and the other residues line the wall of the pocket (Fig. 2). Interestingly, in our structure, the PIF-pocket is occupied by helix αG of a symmetry related molecule (Fig. 2). Tyr288 and Phe291 make hydrophobic contacts in this pocket with almost all pocket-lining residues, remarkably reminiscent of the interactions of the phenylalanines in the FXXF motif in PKA and their hydrophobic docking site in the equivalent region of the kinase domain (Fig. 2). In addition, residues Glu287, Gln292, Ile295 and Lys296 on the symmetry related loop also form contacts with residues lining the PIF-pocket. In total, 244 2 Å of accessible surface is buried by this contact, suggesting this is a tight interaction. However, the significance of this interaction is not clear as an oligomerisation event for PDK1 has not been demonstrated in solution previously. Indeed both the isolated catalytic domain of PDK1 that was crystallised and full length PDK1 migrate in gel filtration chromatography as apparent monomeric species (data not shown).

The phosphate pocket

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As outlined in the introduction, substrates of PDK1, such as S6K1, interact with the PIF-pocket of PDK1 with higher affinity when they are phosphorylated at their hydrophobic motif. This suggested that a regulatory phosphate binding site may be located close to the PIF-pocket. During refinement of the PDK1 structure, it became clear that next to the PIF-pocket another small pocket was present, occupied by a tetrahedral oxyanion (Fig. 2). As 2.0 M of sulphate was present in the crystallisation conditions, this was assigned as a sulphate ion. The ion interacts with four residues lining the pocket, namely Lys76, Arg131, Thr148 and Gln150.

Because of its close proximity to the PIF-pocket (approximately 5Å) it is possible that this sulphate-occupied pocket could represent the binding site for the phosphate on the phosphopeptide. To investigate this further, we mutated Lys76, Arg131, Thr148 and Gln150 to Ala, in order to verify the contribution of each of these residues in enabling PDK1 to interact with a peptide encompassing the hydrophobic motif of S6K1, in which the residue equivalent to Thr412 was phosphorylated (termed S6K-pHM). A quantitative surface plasmon resonance based binding assay (Fig. 4A) showed that wild type PDK1 interacted with S6K-pHM, with a Kd of 0.6 µM with S6K-pHM but not detectably to the non-phosphorylated form of this peptide (S6K-HM). The PDK1[R131A] and PDK1[O150A] mutants did not detectably interact with S6K-pHM in this assay (Fig. 4B). confirming that the interactions these residues make in the PDK1 structure are of key importance. The PDK1[K76A] mutant interacted with 3-fold lower affinity (Kd 1.7 µM) with S6K-pHM. The PDK1[T148A] mutant however possessed about 10-fold higher (Kd 0.06 µM) affinity for S6KpHM than wild type PDK1. Moreover, the dissociation of PDK1[T148A] from S6K-pHM is markedly slower than that of wild type PDK1 or PDK1[K76Al (Fig 4A). These findings are unexpected as Thr148 is within hydrogen bonding distance of the sulphate (Fig. 2), but indicate that this residue may play a role in enabling the dissociation of PDK1 from S6KpHM.

The binding of PDK1 to PIFtide stimulates up to 4-fold the rate at which PDK1 phosphorylates a small peptide that encompasses the activation loop motif of PKB (termed T308tide) [Biondi et al., 2000], indicating that occupancy of the PIF-pocket of PDK1 activates the enzyme. Similarly, the binding of a phosphopeptide corresponding to the hydrophobic motif of RSK stimulated PDK1 activity 6-fold [Frodin et al., 2000]. We have now also found that the binding of S6K-pHM to wild type PDK1 induces a

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maximal 5-fold activation, with a half maximal activation occurring at a concentration of approximately 50 uM S6K-pHM (Fig. 4C). We next assayed the specific activities of PDK1[K76A]. PDK1[R131A]. PDK1[T148A] and PDK1[Q150A] mutants in the absence and presence of increasing concentrations of S6K-pHM (Fig. 4C). The PDK1[K76A] possessed the same specific activity towards T308tide in the absence of S6K-pHM as wild type PDK1, but an approximately 3-fold higher concentration of S6K-pHM was required to half maximally activate PDK1[K76A], consistent with the reduced affinity of this form of PDK1 for S6K-pHM (Fig. 4A,B). The PDK1[R131A] mutant possessed a 3-fold higher specific activity towards Thr308tide in the absence of S6K-pHM (Fig. 4C), as has been observed previously with certain other PIF-pocket mutants of PDK1(PDK1[K115A] and PDK1[L155E]) [Biondi et al., 2000]. However, in accordance with the inability of PDK1[R131A] to bind S6KpHM in the Biacore assay (Fig. 4B), it was not significantly activated by concentrations of S6K-pHM below 0.1 mM and its activity was only moderately further increased by the addition of high concentrations (0.3 and 1 mM) of S6K-pHM (Fig. 4C). The activity of a mutant of PDK1 in which both Lys76 and Arg131 were changed to Ala was activated even less significantly by these high concentrations of S6K-pHM. The PDK1[T148A] and PDK1[Q150A] mutants possessed similar specific activity towards T308tide as wild type PDK1 in the absence of S6K-pHM. PDK1[T148A] mutant was activated similarly as wild type PDK1 by S6KpHM and consistent with the inability of PDK1[Q150A] to interact with S6K-pHM, this mutant of PDK1 was not significantly activated by concentrations of S6K-pHM below 0.1 mM but at 0.3 and 1 mM peptide a 2-3 fold activation was observed (Fig. 4).

At very high peptide concentrations (0.3-1 mM) the non-phosphorylated S6K-HM

peptide induced a small (<2-fold) activation of PDK1 (Fig. 4C). Interestingly, despite the PDK1[K76A] and PDK1[R131A] mutants being markedly less able to interact with the phosphorylated S6K-pHM peptide, than wild type PDK1, high concentrations of the S6K-HM peptide activated PDK1[K76A] and PDK1[R131A] to a similar extent as wild type PDK1, indicating that the ability of these mutants to interact weakly with the S6K-HM peptide was not affected.

We evaluated the sequence conservation in the phosphate pocket of the insulin/growth factor-activated AGC family kinases (PKBa, S6K1, SGK1 and RSK1). Sequence alignments indicate that this pocket is conserved amongst these kinases (Fig 5A). The most conserved residue is Gln150 which is found in all of these AGC kinases and the residue equivalent to Lys76 is always a basic residue (Fig. 5A). Arg131 is conserved in S6K1, SGK1 and RSK1 but not in PKBa, or PKBb or PKBy, where it is an Asn or Ser. Thr148 is conserved in PKBα and SGK1 but is an Ala in S6K1 and RSK1. Interestingly, we have found the Thr 148Ala mutation in PDK1 did not disrupt the phosphate pocket (Fig 4). As PKBα, S6K1, SGK1 and RSK1 require to be phosphorylated at their hydrophobic motif to be maximally activated, it is tempting to speculate that the C-terminal hydrophobic motifs of these enzymes, when phosphorylated, bind to their own PIF/phosphate pockets, thereby generating a network of interactions similar to that of PDK1. In support of this, PKBa, S6K1, SGK1 and RSK1 also require phosphorylation of their activation loop at the position equivalent to Ser241 for activity. Consistent with PKA not possessing a phosphate pocket, Lvs76 and Gln150 are not conserved in PKA (Fig. 3). and indeed such a pocket is not observed in the PKA structure (Fig. 2).

The &C helix

The PDK1 structure shows that, as in other protein kinases [Johnson et al., 2001, Husen and Kuriyan, 2002], the α C helix (residues 124-136) is a key signal integration motif in the kinase core. One turn of the PDK1 α C helix (residues 129-131, Figs. 3, 5) links together the N-terminal lobe, the C-terminal lobe and the active site. Arg129 points towards the activation loop and forms two hydrogen bonds with the phosphorylated Ser241, whereas Arg131 forms two hydrogen bonds with the sulphate in the phosphate pocket (Fig. 5). Glu130 coordinates Lys111 which forms a hydrogen bond with the α -phosphate of the bound ATP. This interaction is conserved in all protein kinases and shown to be crucial for activation [Johnson et al., 2001, Husen and Kuriyan, 2002]. An additional residue, His126, forms a third hydrogen bond with the phosphorylated Ser241. Val124 and Val127 on the α C helix are involved in formation of the PIF-pocket (Fig. 5).

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The αC helix provides a structural link between the putative phosphopeptide binding pocket and the phosphoserine in the activation loop. The fact that R131A has higher basal activity than wild type PDK1 may indicate that this residue plays tuning role in the PDK1 structure, not only participating in the activation of PDK1 in the presence of a phosphate ion, but also on keeping the equilibrium of the enzyme towards an inactive conformation in the absence of S6K-pHM. To our knowledge this is the first report of a kinase structure in which the αC helix is positioned by 2 regulatory phosphate binding sites on either side of the helix (Fig 5). This provides a possible sensor-mechanism for linking the phosphorylation-state of the activation loop and the phosphopeptide binding event in the PIF-pocket to PDK1 activity.

Activation state

All structures of PKA solved to date show a phosphorylated T-loop and are therefore assumed to be in an active state. In addition to the unphosphorylated versus phosphorylated states of PKA, there appear to be two main conformational states possible for the latter [Zheng et al., 1993, Johnson et al., 2001]. In the active, closed conformation, all residues are positioned to facilitate phosphoryl transfer. In contrast, the inactive, open conformation is seen in absence of a nucleotide, and differs from the closed conformation by conformational changes of the N-terminal and C-terminal domains with respect to each other. In addition, three 'intermediate' structures were described from PKA, having either adenosine (PDB entry 1BKX [Narayana et al., 1997]) or the inhibitors staurosporine (PDB entry 1STC [Prade et al., 1997]) and balanol (PDB entry 1BX6 [Narayana et al., 1999]) in the ATP-binding site. Taylor and colleagues have described a method to distinguish between the active and inactive conformations, based on three distances: His87-pThr197 (αC helix positioning), Ser53-Gly186 (opening of the glycine-rich loop) and Glu170-Tyr330 (C-terminal tail distance to active site) [Johnson et al., 2001]. In PDK1, only one of these distances, the opening state of the glycine rich loop, can be measured due to sequence conservation (Fig. 3). This distance is 12.4 Å, similar to a PKA intermediate conformation (this distance in PKA is 14.2Å for the open, 11.8 Å for intermediate and 10.0 Å for the closed conformation [Johnson et al., 2001]). To allow a more direct comparison of the PDK1 structure with the available PKA structures, we have analysed the conformational state of PDK1 in detail using a novel approach, which involves a principal component analysis (also called "essential dynamics" [Amadei et al.,1993]) of the crystallographic coordinates. In short, this involves the construction of a covariance matrix containing the correlations between atomic shifts (with respect to an average structure) in the ensemble of all available PKA crystal structures. Diagonalisation of this matrix gives eigenvector/eigenvalue sets which describe concerted shifts of atoms

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(eigenvectors) together with the corresponding mean square fluctuation of the structures (eigenvalues). This approach allows a condensed description of PKA conformational states using only a few degrees of freedom, as shown previously for a range of other proteins [van Aalten et al., 1997, van Aalten et al., 2000,deGroot et al., 1998]. Diagonalisation of a covariance matrix built from the backbone atoms of residues 37-196, 198-283 and 286-305 results in a set of eigenvectors that describe concerted motions of the PKA backbone. In Fig. 6A, all PKA structures are projected on a subspace spanned by the first two eigenvectors (i.e. those with the two largest eigenvalues). It appears that the PKA structures cluster in three main areas along the first eigenvector. On the left of the average structure (which by definition has a projection of 0.0 on all eigenvectors) are the structures that are known to be in the "open" conformation (Fig. 6A). Around the average structure lie the structures that have been shown to be in an "intermediate" conformation (complexes with the inhibitors staurosporine, balanol and adenosine). More to the right of the average structure are the PKA structures that are known to be in the "closed" conformation. Thus, we have captured the conformational state of PKA in a single variable, the translation along the first eigenvector. This is further clarified by investigation of the atomic shifts described by this eigenvector in Cartesian space (Fig. 6B). A hinge-bending motion is observed between the Nterminal and C-terminal lobes, opening and closing the active site. It is now possible directly to compare the PDK1 conformational state by projecting the structure (backbone atoms only) onto the PKA eigenvectors. Fig. 6A shows that the conformation of PDK1 is close to the PKA structures that are in an "intermediate" conformation, consistent with the other structural analyses described above.

Conclusions

We have reported the structure of the PDK1 catalytic domain, which, although similar to PKA, has revealed important features that increase our understanding of the mechanism by which PDK1 is regulated. The structure, together with mutational analyses, defines a phosphopeptide binding pocket, consisting of a separate hydrophobic PIF-pocket and a phosphate binding site, which mediates the interaction of PDK1 with the phosphorylated hydrophobic motif of S6K. This is consistent with the previous hypothesis that phosphorylation of S6K and SGK [Biondi et al., 2001] as well as RSK [Frodin et al., 2000] at their FXXFS/T hydrophobic motif (SEO ID NO:2) is the trigger for their interaction and phosphorylation by PDK1. In this mechanism the PIF-pocket would physiologically only interact with the Phe residues when the Ser/Thr residue is phosphorylated. Furthermore, as the phosphate pocket is conserved in other AGC kinases, the structural features and network of interaction of the phosphate pocket with the aC-helix on PDK1, could provide insight into the mode of activation of other AGC kinases

Experimental Procedures

20 Materials

Mammalian and Insect cells culture reagents were from Life Technologies. SensorChips SA were from BiaCore AB. Glutathione Sepharose, as well as pre- packed HiTrap Q HP and Hiload Superdex 200 prep grade columns were from Amersham Biosciences. Dialysis cassettes were from the Slide-A-Lyzer series (Pierce). Ni-NTA Agarose was from Qiagen. Disposable ultrafiltration devices (polyethersulfone membranes) were from Vivascience. Crystallisation research tools (primary screens, additive

screens and crystallisation plates) were from Hampton Research. Peptides were synthesised by Dr G. Blomberg (University of Bristol, UK).

General methods

Molecular biology techniques were performed using standard protocols. Site directed mutagenesis was performed using a QuickChange kit (Stratagene) following instructions provided by the manufacturer. DNA constructs used for transfection were purified from bacteria using Qiagen plasmid Mega kit according to the manufacturer's protocol, and their sequence verified. Human kidney embryonic 293 cells were cultured on 10 cm diameter dishes in Dulbecco's modified Eagle's medium containing 10% foetal boying serum.

Buffers

Low Salt Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl; High Salt Buffer: 25mM Tris-HCl pH 7.5, 500 mM NaCl. Lysis Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl 0.07% β -mercaptoethanol, 1mM Benzamidine, and 20 μg/ml PMSF. Buffer A: 50 mM Tris-HCl pH 7.5, 1 mM EGTA, 1 mM EDTA, 1% (by mass) Triton-X 100, 1 mM sodium orthovanadate, 50 mM sodium fluoride, 5 mM sodium pyrophosphate, 0.27 M sucrose, 1 μM microcystin-LR, 0.1% (by vol) β -mercaptoethanol and "complete" proteinase inhibitor cocktail (one tablet per 50 ml, Roche). Buffer B: 50 mM Tris/HCl pH 7.5, 0.1 mM EGTA, 10 mM β -mercaptoethanol and 0.27 M sucrose.

A cDNA encoding for human PDK1 amino acid residues 51-359 with a stop codon inserted at position 360, was amplified by PCR reaction using full length human PDK1 cDNA in the pCMV5 vector [Alessi et al., 1997] as a template a 5'primer, which incorporates a BamH1 restriction site, an initiating methionine, a hexahistidine tag.followed by a PreScission protease recognition sequence prior to the residue equivalent to Met51 of PDK1 (ggatcctataaatatggcacatcatcatcatcatcatctggaagttctgttccaggggcccatggacggcact geageegageetegg) (SEO ID NO:106) and the 3' primer applied in this reaction was: 5'-ggatcctcaggtgagcttcggaggcgtctgctggtg-3' (SEO ID NO: 107). The resulting PCR product was ligated into pCR 2.1 TOPO vector (Invitrogen) and then subcloned as a BamH1-BamH1 fragment into pFastbac1 vector (Life Technologies) for baculovirus protein expression. The resulting construct was then used to generate recombinant baculovirus using the Bac-to-Bac system (Life Technologies) following the manufacturer's protocol. The resulting baculoviruses were used to infect Sf21 cells at 1.5 x 106/ml. The infected cells were harvested by centrifugation 72 hours post infection. Cell pellets corresponding to 7 l of culture were resuspended in 900 ml of Lysis Buffer and cells lysed in nitrogen cavitation chamber. Cell debris was then pelleted by centrifugation, the supernatant made 0.5 M NaCl by addition of 4M NaCl and then incubated with Ni-NTA-Agarose (10 ml resin) for one hour. The resin was then washed in 10 times with 40 ml of Lysis Buffer containing 0.5M NaCl and then placed in a disposable Econo-Pac column (BioRad), where the resin was further washed with 700 ml of high salt buffer and then with 100 ml of low salt buffer, both supplemented with 10 mM imidazole. Elution was performed with 200 mM imidazole in high salt buffer and 2 ml fractions were collected. Fractions containing protein were pooled, diluted to 200 mM NaCl with 25 mM Tris/HCl pH 7.5, and loaded onto a 5 ml Hitrap O sepharose column. The flow-through from this step, containing PDK1, was concentrated to 4 ml and then chromatographed on a 16/60

Superdex 200 gel filtration column using an AKTA Explorer system (Amersham Biosciences) equilibrated with high salt buffer with the addition of 1mM DTT. PDK1 eluted in a large symmetric peak at the expected size for a monomer. The PDK1 containing peak was again pooled, concentrated and incubated with 300 μg GST-PreScission protease (expression construct kindly provided by John Heath, University of Birmingham, UK) on ice for 4h. In order to eliminate the cleaved His-tag sequences as well as any remaining uncleaved His-PDK1 and the GST-PreScission protease, the mixture was incubated with a mixture of 200 μl glutathione-Sepharose and 200 μl Ni-NTA agarose resin for 15 minutes and the PDK1 protein that did not bind was collected. The resulting protein consists of PDK1 (51-359) preceded by a Gly-Pro at the N-terminus. The protein at this stage of the purification was apparently homogeneous as revealed by a single band after electrophoresis of 20 μg of protein on SDS-PAGE and staining with Coomasie Brilliant Blue R250 (data not shown).

Electrospray mass spectrometry revealed a main peak mass close to the expected size of this fragment of PDK1. The specific activity of PDK1 (51-359) towards the peptide T308tide and its activation in the presence of PIFtide was identical to wild type full length PDK1 [Biondi et al., 2000], and tryptic peptide mass finger printing indicated that PDK1 was quantitatively phosphorylated at Ser241 (data not shown). In BiaCore experiments, the steady state binding of PDK1 (51-359) to the peptide PIFtide was similar to that of the His-tag PDK1 (51-556) protein characterised previously [Balendran et al., 1999a].

Crystallisation and data collection

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The PDK1 (51-359) protein was concentrated to a final concentration of 8.5 mg/ml (as determined by a Bradford assay using bovine serum albumin as a standard). The sitting drop vapour diffusion method was used for producing crystals. Sitting drops were formed by mixing 1 µl of protein solution with 1 µl of a mother liquor solution (0.1 M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP) with the addition of 0.2 µl EDTA (100mM). Hexagonal crystals (Table I) of PDK1 were grown at 20° C from a mother liquor containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP). Crystals appeared after one day, growing to 0.05 x 0.05 x 0.2 mm over 20 days. Crystals were frozen in a nitrogen gas stream after being soaked in 0.075 M Tris 8.5, 1.5M ammonium sulphate, 25% (v/v) glycerol.

Expression and purification of wild type and mutant forms of GST-PDK1.

Wild type-PDK1 [Alessi et al., 1997], PDK1[R76A], PDK1[R131A], PDK1[R76A,R131A], PDK1[T148A] and PDK1[Q150A] in the pEBG2T vector were used to express the wild type and indicated mutants of PDK1 fused through their N-terminus to glutathione S-transferase (GST). The GST fusion proteins were expressed in human embryonic kidney 293 cells. For the expression of each construct, twenty 10 cm diameter dishes of 293 cells were cultured and each dish transfected with 10 μg of the pEBG-2T construct, using a modified calcium phosphate method. 36 h post-transfection, the cells were lysed in 0.6 ml of ice-cold Buffer A, the lysates pooled, centrifuged at 4 ° C for 10 min at 13000 g and the GST-fusion proteins were purified by affinity chromatography on glutathione-Sepharose and eluted in Buffer B supplemented with 20 mM glutathione as described previously [Alessi et al., 1997]. Typically between 1 and 2mg of each GST-fusion protein was obtained and each protein was more than 75 judged by SDS polyacrylamide gel electrophoresis (data not shown).

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PDK1 catalytic activity measurements

The ability of wild type and mutant PDK1 to phosphorylate the synthetic peptide T308tide (KTFCGTPEYLAPEVRR ([Biondi et al., 2000]) (SEQ ID NO:108) was carried out in 30 ul assays containing 100 ng of wild type or mutant PDK1, 50 mM Tris/HCl pH 7.5, 0.1% B -mercaptoethanol, 10 mM MgCl₂, 100 µM [32\gamma PlATP (200 cpm/pmol) , 0.5 µM microcvstin-LR, 1 mM T308tide in the presence or absence of the indicated concentrations of the S6K-pHM peptide (SESANQVFLGFT(P)YVAPSV) (SEQ ID NO:104) or S6K-HM.peptide (SESANQVFLGFTYVAPSV) (SEQ ID NO:105). After incubation for 10 min at 30 °C, 25 µl of the resultant mixture was spotted into P81 phosphocellulose paper (2 x 2 cm) and the papers washed and analysed as described previously for assays of MAP kinase. Control assays were carried out in parallel in which either PDK1, or peptide substrate were omitted; these values were always less than 5% of the activity measured in the presence of these reagents. One Unit of PDK1 activity was defined as that amount required to catalyse the phosphorylation of 1 nmol of the T308tide in 1 min

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Biacore analysis

Binding was analysed in a BiaCore 3000 system (BiaCore AB, Stevenage, UK). Biotinylated S6K-pHM (Biotin-C₁₂- SESANQVFLGFT(P)YVAPSV) (SEQ ID NO:104) or the non-phosphorylated form of this peptide S6K-HM was bound to an streptavidin- coated Sensor chip (SA) (12 response units, RU). 30 μl of wild type or the indicated mutant GST-PDK1 were injected at a flow rate of 30μl/min, in buffer HBS-P (10 mM HEPES pH 7.4, 0.15M

NaCl, 0.005% (by vol) polysorbate-20) supplemented with 1 mM DTT. Specific interactions between S6K-pHM and PDK1 proteins were obtained between the concentration range of 2-2150 nM PDK1. Steady state binding was determined at each concentration. Dissociation of PDK1 from the phospho-peptide was monitored over a 1min period. Regeneration of the sensor chip surface was performed with 10µl injections of 0.05% SDS. As previously found for PDK1 binding to PIFtide [Biondi et al., 2000], the interaction data obtained using BiaCore did not fit to simple 1:1 interaction model. Apparent Kd values were estimated from the concentration of PDK1 which gives 50% of maximal response, which was obtained empirically using GST- PDK1[T148A] (RUmax=435). For all PDK1 construct tested. the off rates for S6Kp-HM were high in comparison to those of PIFtide binding with the time taken for 50% dissociation to occur for S6K-pHM is 30s compared to 1000s for PIFtide. This could account for the overall approximately 100-fold lower affinity of wild type PDK1 for S6K-pHM in comparison to PIFtide.

Data collection, structure solution, and refinement

Data on PDK1 crystals were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH1, using an ADSC Q4 CCD detector. The temperature of the crystals was maintained at 100K using a nitrogen cryostream. Data were processed using the HKL package [Otwinowski and Minor, 1997], statistics are shown in Table I.

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The structure of PDK1 was solved by molecular replacement with AMoRe [Navaza, 1994] using the structure of PKA in complex with an inhibitory peptide as a search model (PDB entry 1YDB), against 8-4 Ådata. A single, well separated solution was found with an R-factor of 0.479 (correlation

coefficient = 0.428). The structure was automatically built using warpNtrace [Perrakis et al., 1999], which found 262 of a possible 309 residues, giving an initial protein model with R=0.293 (Rfree=0.318) after simulated annealing in CNS [Brunger et al., 1998]. Iterative protein building in O [Jones et al., 1991] together with refinement in CNS, which included incorporation of a model for ATP, the phosphoserine in the activation loop, solvent molecules and a key sulphate molecule, resulted in a final model with R=0.195 (Rfree=0.222). No electron density was observed for residues 51-70 (the N-terminus of the construct) and 233-236 (the tip of the activation loop). All figures were made with PyMOL.

Table I

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Details of data collection & structure refinement for the PDK1 kinase domain. Values between brackets are for the highest resolution shell. All measured data were included in structure refinement.

Wave length ()	0.933
Space group	P3 ₂ 21
Unit cell ()	a=123.01, b=123.01, c=47.62
Resolution ()	25-2.0 (2.07-1.0)
Observed reflections	77315
Unique reflections	27643
Redundancy	2.8 (2.5)
Completeness(%)	98.0 (93.5)
Rmerge	0.091 (0.454)
I/ sigma I	7.3 (2.0)
R _{free} reflections	579
R _{cryst}	0.195
R _{free}	0.222

	Number of groups	
	°°Protein residues	71-359
	°°Water	200
	ATP	1
5	SO ₄	5
	Glycerol	8
	Wilson B (2)	22.4
	< B > Protein	25.6
	< B > Water	35.7
10	< B > ATP	38.8
	RMSD from ideal geometry	
	Bond lengths ()	0.005
	Bond angles (°)	1.34
	Main chain B (2)	1.5.

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Example 2: Co-ordinates for PDK1fragment with all alternate side chains.

```
REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.0 A
    REMARK starting r= 0.1972 free r= 0.2220
   REMARK final
                  r= 0.1954 free r= 0.2224
    REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
   REMARK rweight= 0.0900 (with wa= 1.29263)
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1 : /ddl/david/projects/PDK1 new/CNS/prot.par
   REMARK parameter file 2 : /ddl/david/projects/PDK1_new/CNS/atp.par
    REMARK parameter file 3 : CNS TOPPAR:water rep.param
    REMARK parameter file 4 : CNS_TOPPAR:ion.param

REMARK parameter file 5 : /ddl/david/projects/PDK1 new/CNS/glycerol.par
    REMARK molecular structure file: ../generate/alternate.mtf
   REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../1/hkl/cns.hkl
    REMARK nos= none
    REMARK B-correction resolution: 6.0 - 2.0
    REMARK initial B-factor correction applied to fobs :
   REMARK B11= -2.766 B22= -2.766 B33= 5.532
REMARK B12= -0.375 B13= 0.000 B23= 0.000
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    REMARK B-factor correction applied to coordinate array B: 0.031
    REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
    REMARK reflections with |Fobs|/sigma F < 0.0 rejected
   REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range:
                                                                   28210 ( 100.0
    % )
    REMARK number of unobserved reflections (no entry or |F|=0):
                                                                     568 (
                                                                             2.0
   REMARK number of reflections rejected:
                                                                       0 (
                                                                             0.0
    REMARK total number of reflections used:
                                                                   27642 ( 98.0
    REMARK number of reflections in working set:
                                                                   27063 ( 95.9
40
    REMARK number of reflections in test set:
                                                                     579 ( 2.1
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              1 CB PRO A 71
                                 58.912 -7.251 8.216 1.00 67.78
    ATOM
              2 CG PRO A 71
                                59.621 -6.941 9.534 1.00 69.16 A
                                59.493 -6.506 5.894 1.00 67.06 A
    ATOM
              3 C
                    PRO A 71
   ATOM
              4 O PRO A 71
                                59.196 -5.318 5.766 1.00 66.66 A
    ATOM
              5 N PRO A 71
                                60.984 -6.073 7.833 1.00 67.86 A
    MOTA
              6 CD PRO A 71
                                60.554 -5.762 9.207 1.00 68.24 A
              7 CA PRO A 71
                                 60.040
                                         -7.035
                                                 7.217 1.00 67.75 A
    MOTA
             8 N PRO A 72
                                 59.356 -7.385 4.890 1.00 66.32 A
    MOTA
    MOTA
              9 CD PRO A 72
                                59.712
                                         -8.816
                                                 4.898 1.00 67.17 A
             10 CA PRO A 72
                                58.840 -6.986 3.578 1.00 65.61 A
    ATOM
            11 CB PRO A 72
                                58.672 -8.321 2.858 1.00 66.47 A
    MOTA
            12 CG PRO A 72
                                59.796 -9.133 3.419 1.00 67.57 A
    MOTA
```

	ATOM	13	C	PRO			-6.208	3.673	1.00 63.94	Α
	ATOM	14	0	PRO			-6.451	4.561	1.00 64.11	A
	MOTA	15	N	ALA	A 7	3 57.341	-5.268	2.753	1.00 61.57	A
	MOTA	16	CA	ALA	A 7	3 56.133	-4.454	2.708	1.00 58.74	A
5	ATOM	17	CB	ALA	A 7	3 56.438	-3.030	3.165	1.00 58.05	A
	ATOM	18	C	ALA	A 7	3 55.626	-4.448	1.271	1.00 56.78	A
	ATOM	19	0	ALA	A 7	3 56.347	-4.834	0.349	1.00 56.95	A
	ATOM	20	N	PRO			-4.024	1.057	1.00 54.15	A
	ATOM	21	CD	PRO			-3.610	2.018	1.00 53.31	A
10	ATOM	22	CA	PRO			-4.003	-0.314	1.00 52.54	A
	ATOM	23	CB	PRO			-3.375	-0.148	1.00 52.86	A
	ATOM	24	CG	PRO			-3.824	1.226	1.00 52.88	A
	ATOM	25	C	PRO			-3.167	-1.204	1.00 50.08	A
	ATOM	26	o	PRO			-2.361	-0.708	1.00 49.96	A
15	ATOM	27	N	ALA			-3.366	-2.514	1.00 47.58	A
	ATOM	28	CA	ALA			-2.602	-3.446	1.00 44.69	A
	ATOM	29	CB	ALA			-3.121	-4.870	1.00 46.14	A
	ATOM	30	CB	ALA			-1.134	-3.371	1.00 41.55	A
							-0.813			
20	ATOM	31	0	ALA				-3.086 -3.619	1.00 41.01	A
20	ATOM	32	N				-0.245	-3.588	1.00 35.31	A
	ATOM	33	CA	LYS			1.184			A
	ATOM	34	CB	LYS			1.957	-3.930	1.00 37.70	A
	ATOM	35	CG	LYS			3.356		1.00 40.99	A
2.5	MOTA	36	CD	LYS			3.316	-1.836	1.00 40.04	A
25	MOTA	37	CE	LYS			4.705	-1.277	1.00 42.08	A
	MOTA	38	NZ	LYS			4.695	0.202	1.00 42.99	A
	ATOM	39	C	LYS			1.467	-4.638	1.00 32.65	A
	MOTA	40	0	LYS			1.005	-5.770	1.00 31.41	A
	MOTA	41	N	LYS			2.207	-4.270	1.00 28.59	A
30	MOTA	42	CA	LYS			2.517	-5.232	1.00 25.72	A
	MOTA	43	CB	LYS			2.865	-4.509	1.00 26.22	A
	ATOM	44	CG	LYS			1.731	-3.631	1.00 27.15	A
	MOTA	45	CD	LYS			2.089	-2.967	1.00 26.80	A
	MOTA	46	CE	LYS			1.091		1.00 27.31	A
35	ATOM	47	NZ	LYS			-0.296		1.00 27.17	A
	ATOM	48	C	LYS			3.668	-6.137	1.00 24.67	A
	MOTA	49	0	LYS			4.377	-5.829	1.00 21.60	A
	MOTA	50	N	ARG			3.838	-7.254	1.00 23.66	A
	ATOM	51	CA	ARG	A 7	52.662	4.897	-8.211	1.00 26.14	A
40	ATOM	52	CB	ARG	A 7	53.574	4.344	-9.318	1.00 28.57	A
	ATOM	53	CG	ARG	A 7:	53.017	3.139	-10.050	1.00 34.78	A
	MOTA	54	CD	ARG	A 7	54.092	2.465	-10.896	1.00 40.96	A
	ATOM	55	NE	ARG	A 7	53.560	1.364	-11.700	1.00 48.93	A
	ATOM	56	CZ	ARG	A 7	52.985	0.270	-11.203	1.00 52.58	A
45	ATOM	57	NH1	ARG	A 7	52.860	0.113	-9.889	1.00 54.60	A
	MOTA	58	NH2	ARG	A 7	52.530	-0.672	-12.022	1.00 54.09	A
	MOTA	59	С	ARG	A 7	51.382	5.488	-8.803	1.00 23.76	A
	ATOM	60	0	ARG	A 7	50.311	4.888	-8.706	1.00 24.25	A
	MOTA	61	N	PRO	A 7	51.475	6.676	-9.428	1.00 21.76	A
50	MOTA	62	CD	PRO	A 7	52.691	7.475	-9.668	1.00 20.82	A
	MOTA	63	CA	PRO	A 7	50.301	7.325	-10.021	1.00 21.96	A
	ATOM	64	CB	PRO				-10.816	1.00 22.27	A
	ATOM	65	CG	PRO			8.831	-10.014	1.00 22.12	A
	ATOM	66	c	PRO				-10.903	1.00 22.86	
55	ATOM	67	0	PRO				-10.842	1.00 20.52	A
	MOTA	68	N	GLU				-11.714	1.00 21.87	A
	ATOM	69	CA	GLU				-12.628	1.00 22.99	A
	ATOM	70	CB	GLU		50.393	3.994 -			AC1
	ATOM	71	CG	GLU		51.230	2.907 -			AC1
					-					

	ATOM	72	CD	GLU		80	52.157	2.2	24 -1	3.9	13	0.50	31.9	9 AC1	
	ATOM	73	OE1	GLU		80	53.072	2.8	97 -1	4.4	33	0.50	34.3	4 AC1	
	ATOM	74	OE2	GLU		80	51.969	1.0	15 -1	4.1	.72	0.50	32.8	3 AC1	
	ATOM	75	C	GLU	A	80	48.556	3	.631	-11			00 22		
5	ATOM	76	ō	GLU		80	47.692		.013				00 22		
	ATOM	77	N	ASP		81	48.804		.413				00 19		
	ATOM	78	CA	ASP		81	48.026		.423		.874		00 19		
	ATOM	79	CB	ASP		81	48.736		.029		.571		00 21		
	ATOM	80	CG	ASP		81	50.089		.380		.807		00 22		
10	ATOM	81		ASP		81	50.195		.554		.731		00 24		
10															
	ATOM	82		ASP		81	51.		1.6		-8.			23.33	A
	ATOM	83	С	ASP		81	46.		2.9		-9.			20.85	A
	MOTA	84	0	ASP		81	45.		2.2		-9.			19.96	A
	MOTA	85	N	PHE		82	46.		4.2		-9.			18.91	A
15	MOTA	86	CA		A	82	45.		4.9		-9.			19.30	A
	MOTA	87	CB		А	82	45.		6.0		-8.			18.43	A
	MOTA	88	CG	PHE	Α	82	46.	134	5.5		-7.		1.00	18.01	A
	MOTA	89			Α	82	45.	371	5.1	.36	-6.		1.00	17.19	A.
	MOTA	90	CD2	PHE	Α	82	47.	520	5.4	60	-7.	086	1.00	18.99	A.
20	MOTA	91	CE1	PHE	Α	82	45.	977	4.6	76	-4.	918	1.00	17.12	A
	ATOM	92	CE2	PHE	Α	82	48.	137	5.0	0.0	-5.	925	1.00	19.64	A
	ATOM	93	CZ	PHE	A	82	47.	361	4.6	07	-4.	838	1.00	18.00	A
	ATOM	94	C	PHE	A	82	44.	476	5.5	96	-10.	621	1.00	20.81	A
	ATOM	95	0	PHE	А	82	45.	066	5.9	33	-11.	649	1.00	20.34	A
25	ATOM	96	N	LYS		83	43.				-10.			19.80	A
	ATOM	97	CA	LYS		83	42.				-11.			21.65	A
	ATOM	98	CB	LYS		83	41.				-11.			22.02	A
	ATOM	99	CG	LYS		83	40.				-12.			28.93	A
	ATOM	100	CD	LYS		83	38.				-12.			34.20	A
30	ATOM	101	CE	LYS		83	37.				-13.			38.10	A
30	ATOM	102	NZ	LYS		83	37.				-13.			43.33	A A
	ATOM	102	C	LYS		83	41.				-10.			20.74	A A
	ATOM	104	0	LYS		83	41.		7.6		-9.			20.98	A
	MOTA	105	N		A	84	42.				-10.			19.99	A
35	MOTA	106	CA		A	84	42.				-10.			18.63	A
	ATOM	107	CB	PHE		84	43.				-10.			18.95	A
	MOTA	108	CG	PHE		84	44.		10.7		-9.			17.68	A
	MOTA	109			Α	84	45.				-10.			18.16	A
	MOTA	110		PHE		84	44.	843	11.1		-8.	299	1.00	19.66	A.
40	MOTA	111	CE1	PHE	A	84	46.	676	9.5	56	-9.	589	1.00	18.09	A.
	MOTA	112	CE2	PHE	A	84	46.	021	10.8	16	-7.	653		18.89	A
	MOTA	113	CZ	PHE	A	84	46.	936	10.0	02	-8.	301	1.00	17.33	A
	ATOM	114	C	PHE	A	84	40.	834	10.6	17	-10.	460	1.00	19.69	A
	ATOM	115	0	PHE	A	84	40.	391	10.4	89	-11.	601	1.00	20.72	A
45	ATOM	116	N	GLY	A	85	40.	178	11.2	33	-9.	484	1.00	16.80	A
	ATOM	117	CA	GLY	A	85	38.	872	11.8	10	-9.	716	1.00	17.73	A
	ATOM	118	С	GLY	А	85	38.	819	13.2	80	-9.	346	1.00	18.75	A
	ATOM	119	0	GLY		85	39.	740	14.0		-9.	650		18.45	A
	ATOM	120	N	LYS		86	37.		13.6		-8.			16.00	A
50	ATOM	121	CA	LYS		86	37.		15.0		-8.			18.26	A
	ATOM	122	СВ	LYS		86	36.		15.3		-7.			19.00	A
	ATOM	123	CG	LYS		86	35.		14.6		-6.			21.55	A
	ATOM	124	CD	LYS		86	34.		14.9		-6.			26.48	A
	ATOM	124	CE	LYS		86	33.		14.2		-4.			31.92	A A
55		125	NZ	LYS			32.		14.4		-4.			35.36	A A
,,	ATOM					86									
	ATOM	127	C	LYS		86	38.		15.5		-7.			18.57	A
	ATOM	128	0		Α	86	39.		14.8		-6.			16.77	A
	MOTA	129	N	ILE		87	38.		16.8		-7.			17.88	A
	ATOM	130	CA	ILE	Α	87	39.	577	17.5	54	-6.	256	1.00	18.26	A

	ATOM	131	CB	ILE	Α	87	39.994	18.952	-6.772	1.00 19.60	A
	ATOM	132	CG2	ILE	A	87	40.593	19.786	-5.628	1.00 18.73	A
	ATOM	133	CG1	ILE	Δ	87	40.968	18.786	-7.945	1.00 21.16	A
	ATOM	134			A	87	41.412	20.087	-8.588	1.00 25.26	A
-											
5	ATOM	135	C	ILE		87	38.731	17.709	-4.997	1.00 19.67	A
	MOTA	136	0	ILE	A	87	37.628	18.249	-5.052	1.00 20.41	A
	ATOM	137	N	LEU	A	88	39.240	17.229	-3.867	1.00 19.15	A
	ATOM	138	CA	LEU	A	88	38.508	17.324	-2.611	1.00 20.68	A
	ATOM	139	CB	LEU		88	38.870	16.151	-1.700	1.00 19.97	A
10	ATOM	140	CG	LEU		88	38.529	14.759	-2.237	1.00 19.24	A
10											
	MOTA	141		LEU		88	39.090	13.692	-1.311	1.00 21.41	A
	ATOM	142		LEU		88	37.029	14.622	-2.359	1.00 18.84	A
	MOTA	143	C	LEU	A	88	38.815	18.632	-1.901	1.00 23.11	A
	ATOM	144	0	LEU	A	88	37.999	19.146	-1.139	1.00 25.10	A
15	ATOM	145	N	GLY		89	39.997	19.174	-2.149	1.00 24.09	A
	ATOM	146	CA	GLY		89	40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	C	GLY		89	41.658	20.954	-2.078	1.00 25.47	A
	MOTA	148	0	GLY		89	42.445	20.202	-2.666	1.00 22.19	A
	ATOM	149	N	GLU	A	90	41.870	22.254	-1.906	1.00 26.22	A
20	ATOM	150	CA	GLU	A	90	43.064	22.924	-2.404	1.00 29.96	A
	ATOM	151	CB	GLU	Α	90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU	D.	90	42.267	23.038	-4.831	1.00 34.32	A
	ATOM	153	CD	GLU		90	41.711	23.930	-5.927	1.00 38.27	A
	ATOM	154		GLU	A	90	40.590	24.456	-5.764	1.00 40.57	A
2.5											
25	MOTA	155	OE2	GLU		90	42.398	24.110	-6.952	1.00 40.90	A
	MOTA	156	C	GLU		90	43.711	23.768	-1.313	1.00 30.68	A
	MOTA	157	0	GLU	A	90	43.049	24.574	-0.668	1.00 32.83	A
	MOTA	158	N	GLY	A	91	45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY	Α	91	45.724	24.332	-0.104	1.00 29.40	A
30	ATOM	160	С	GLY	А	91	46.795	25.151	-0.798	1.00 29.98	A
	ATOM	161	ō	GLY		91	46.894	25.130	-2.028	1.00 28.16	A
	ATOM	162	N	SER		92	47.605	25.870	-0.029	1.00 28.30	A
	MOTA	163	CA	SER		92	48.653	26.681	-0.633	1.00 30.50	A
	MOTA	164	CB	SER		92	49.165	27.717	0.370	1.00 32.43	A
35	ATOM	165	OG	SER	A	92	49.520	27.099	1.593	1.00 40.94	A
	ATOM	166	C	SER	A	92	49.815	25.843	-1.164	1.00 29.77	A
	ATOM	167	0	SER	A	92	50.456	26.221	-2.143	1.00 30.46	A
	MOTA	168	N	PHE	А	93	50.087	24.703	-0.536	1.00 27.65	A
	ATOM	169	CA	PHE	Δ	93	51.185	23.855	-0.995	1.00 26.34	A
40	ATOM	170	CB	PHE		93	52.281	23.785	0.068	1.00 27.95	A
40	ATOM	171	CG	PHE		93	52.861	25.117	0.406	1.00 31.06	A
	MOTA	172		PHE		93	52.283	25.909	1.392	1.00 29.96	A
	ATOM	173		PHE		93	53.949	25.613	-0.308	1.00 31.38	A
	MOTA	174		PHE		93	52.779	27.181	1.665	1.00 32.69	A
45	MOTA	175	CE2	PHE	A	93	54.452	26.883	-0.044	1.00 32.63	A
	ATOM	176	CZ	PHE	A	93	53.864	27.670	0.945	1.00 31.81	A
	MOTA	177	С	PHE	А	93	50.759	22.445	-1.365	1.00 25.39	A
	ATOM	178	ō	PHE		93	51.601	21.559	-1.522	1.00 24.59	A
	ATOM	179	N	SER		94	49.457	22.235	-1.519	1.00 23.63	A
50						94					
30	MOTA	180	CA	SER			48.965	20.912	-1.860	1.00 21.43	A
	MOTA	181	CB	SER		94	49.017	20.013	-0.628	1.00 21.42	A
	ATOM	182	OG	SER	Α	94	48.091	20.475	0.340	1.00 21.19	A
	ATOM	183	C	SER	A	94	47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	0	SER	Α	94	46.795	21.882	-2.173	1.00 18.76	A
55	ATOM	185	N	THR		95	47.174	19.832	-3.038	1.00 19.38	A
	ATOM	186	CA	THR		95	45.840	19.637	-3.580	1.00 17.98	A
	ATOM	187	CB	THR		95	45.818	19.818	-5.110	1.00 19.25	A
	ATOM	188		THR		95	46.196	21.162	-5.434	1.00 22.04	A
	MOTA	189	CG2	THR	A	95	44.421	19.549	-5.661	1.00 17.61	A

	ATOM	190	C	THR		9.5	45.455	18.201	-3.243		18.61	A
	ATOM	191	0	THR	Α	95	46.212	17.264	-3.524	1.00	17.10	A
	ATOM	192	N	VAL	Α	96	44.295	18.024	-2.623	1.00	16.53	A
	ATOM	193	CA	VAL	А	96	43.845	16.685	-2.266	1.00	16.05	A
5	ATOM	194	CB	VAL		96	43.170	16.672	-0.886		16.32	A
,		195		VAL		96	42.741	15.249				
	MOTA								-0.532		18.02	A
	MOTA	196		VAL		96	44.145	17.206	0.168		16.69	A
	ATOM	197	C	VAL		96	42.875	16.207	-3.335		16.42	A
	MOTA	198	0	VAL		96	41.906	16.892	-3.665		16.47	A
10	MOTA	199	N	VAL	Α	97	43.157	15.033	-3.888	1.00	16.80	A
	ATOM	200	CA	VAL	Α	97	42.338	14.471	-4.949	1.00	16.72	A
	ATOM	201	CB	VAL	Α	97	43.153	14.354	-6.255	1.00	18.43	A
	ATOM	202	CG1	VAL		97	42.249	13.927	-7.404		19.69	A
	ATOM	203		VAL		97	43.831	15.685	-6.569		17.84	A
15	ATOM	204	C	VAL		97	41.812	13.091	-4.583		16.77	A
15	ATOM	205	Ö	VAL		97	42.532	12.270	-4.014		17.13	A
	MOTA	206	N	LEU		98	40.545	12.845	-4.895		16.62	A
	ATOM	207	CA	LEU		98	39.947	11.548	-4.624		17.04	A
	ATOM	208	CB	LEU	Α	98	38.424	11.633	-4.743	1.00	16.89	A
20	MOTA	209	CG	LEU	Α	98	37.635	10.342	-4.508	1.00	19.46	A
	ATOM	210	CD1	LEU	Α	98	37.990	9.762	-3.146	1.00	20.07	A
	ATOM	211	CD2	LEU	Α	98	36.143	10.627	-4.588	1.00	17.93	A
	ATOM	212	С	LEU		98	40.512	10.597	-5.677	1.00	17.38	A
	ATOM	213	ō	LEU		98	40.527	10.920	-6.863		18.60	A
25	ATOM	214	N	ALA		99	40.995	9.438	-5.246		17.13	A
23	ATOM	215	CA	ALA		99	41.570	8.466	-6.168		18.42	A
	MOTA	216	CB	ALA		99	43.090	8.524	-6.105		14.76	A
	MOTA	217	С	ALA		99	41.102	7.055	-5.848		21.40	A
	ATOM	218	0	ALA		99	40.941	6.691	-4.679		22.52	A
30	ATOM	219	N	ARG	Α	100	40.878	6.261	-6.888	1.00	19.77	A
	ATOM	220	CA	ARG	Α	100	40.459	4.884	-6.693	1.00	20.85	A
	ATOM	221	CB	ARG	Α	100	39.202	4.585	-7.518	1.00	24.22	A
	ATOM	222	CG	ARG	А	100	38.608	3.205	-7.256	1.00	31.78	A
	ATOM	223	CD	ARG			37.326	2.979	-8.048		36.24	A
35	ATOM	224	NE	ARG			36.213	3.818	-7.594		41.40	A
33	ATOM	225	CZ	ARG			35.566	3.662	-6.439		42.05	A
	MOTA	226		ARG			35.912	2.696	-5.598		40.67	A
	MOTA	227		ARG			34.559	4.468	-6.128		43.65	A
	MOTA	228	C	ARG			41.613	3.985	-7.129		18.63	A
40	ATOM	229	0	ARG			42.078	4.065	-8.271		19.49	A
	MOTA	230	N	GLU	Α	101	42.102	3.157	-6.212	1.00	16.43	A
	MOTA	231	CA	GLU	Α	101	43.196	2.246	-6.533	1.00	16.11	A
	ATOM	232	CB	GLU	Α	101	43.774	1.637	-5.248	1.00	16.79	A
	ATOM	233	CG	GLU	Α	101	44.917	0.657	-5.488	1.00	16.51	A
45	ATOM	234	CD	GLU			45.501	0.115	-4.200		18.20	A
	ATOM	235	OE1	GLU			44.733	-0.081	-3.239		18.32	A
	ATOM	236		GLU			46.725	-0.132	-4.150		17.14	A
	ATOM	237	C	GLU			42.625	1.152	-7.442		17.92	A
50	ATOM	238	0	GLU			41.681	0.462	-7.069		18.02	A
50	MOTA	239	N	LEU			43.198	1.002	-8.632		19.06	A
	ATOM	240	CA	LEU			42.718	0.025	-9.607		20.71	A
	ATOM	241	CB	LEU	Α	102	43.569	0.097	-10.878	1.00	23.42	A
	ATOM	242	CG	LEU	Α	102	43.531	1.426	-11.642	1.00	25.30	A
	ATOM	243	CD1	LEU	Α	102	44.577	1.414	-12.748	1.00	27.88	A
55	ATOM	244	CD2	LEU	Α	102	42.140		-12.214		26.79	A
	ATOM	245	С	LEU			42.671	-1.418	-9.125		21.62	A
	ATOM	246	ŏ	LEU			41.668	-2.103	-9.305		21.09	A
	ATOM	247	N	ALA			43.753	-1.874	-8.507		19.38	A
	ATOM							-3.249				
	ALOM	248	CA	ALA	М	103	43.836	-3.249	-8.035	1.00	20.87	A

	ATOM	249	CB	ALA A		45.284	-3.571	-7.671	1.00		A
	ATOM	250	C	ALA A	. 103	42.919	-3.629	-6.872	1.00	19.92	A
	ATOM	251	0	ALA A	103	42.703	-4.815	-6.628	1.00	20.38	A
	MOTA	252	N	THR A	104	42.361	-2.643	-6.175	1.00	18.12	A
5	ATOM	253	CA	THR A	104	41.517	-2.927	-5.018	1.00	17.15	A
	MOTA	254	CB	THR A	104	42.212	-2.484	-3.717	1.00	19.54	A
	ATOM	255	OG1	THR A	104	42.456	-1.070	-3.773	1.00	19.26	A
	ATOM	256	CG2	THR A	104	43.536	-3.219	-3.529	1.00	17.02	A
	ATOM	257	C	THR A	104	40.159	-2.247	-5.026	1.00	19.44	A
10	ATOM	258	0	THR A	104	39.259	-2.648	-4.285	1.00	18.70	A
	ATOM	259	N	SER A	105	40.034	-1.207	-5.847	1.00	19.65	A
	ATOM	260	CA	SER A		38.819	-0.400	-5.967	1.00		A
	ATOM	261	CB	SER	105	37.598	-1.304	-6.173	0.50	21.81	AC1
	ATOM	262	OG	SER	105	36.431	-0.539	-6.412	0.50	23.01	AC1
15	ATOM	263	C	SER A	105	38.644	0.447	-4.701	1.00	18.99	A
	ATOM	264	0	SER A	105	37.602	1.070	-4.488	1.00	18.66	A
	ATOM	265	N	ARG A	106	39.674	0.468	-3.861	1.00	16.84	A
	ATOM	266	CA	ARG A		39.655	1.267	-2.634	1.00		A
	ATOM	267	CB	ARG A		40.827	0.886	-1.723	1.00		A
20	ATOM	268	CG	ARG A		40.619	-0.367	-0.906	1.00		A
	ATOM	269	CD	ARG A	106	41.887	-0.755	-0.170	1.00	17.43	A
	ATOM	270	NE	ARG A	106	41.620	-1.792	0.824	1.00	20.47	A
	ATOM	271	CZ	ARG A	106	42.548	-2.568	1.371	1.00	20.24	A
	ATOM	272		ARG A		43.821	-2.433	1.017	1.00		A
25	ATOM	273		ARG A		42.198	-3.468	2.285	1.00		A
	ATOM	274	C	ARG A	106	39.785	2.746	-2.981	1.00	17.37	A
	ATOM	275	0	ARG A	106	40.514	3.103	-3.902	1.00	17.75	A
	ATOM	276	N	GLU A	107	39.085	3.599	-2.240	1.00	16.06	A
	ATOM	277	CA	GLU A	107	39.156	5.039	-2.461	1.00	20.80	A
30	ATOM	278	CB	GLU A	107	37.779	5.694	-2.337	1.00	22.93	A
	ATOM	279	CG	GLU A	107	36.711	5.171	-3.269	1.00	30.87	A
	ATOM	280	CD	GLU A	107	35.431	5.975	-3.148	1.00	32.40	A
	ATOM	281	OE1	GLU A	107	35.262	6.939	-3.923	1.00	33.74	A
	ATOM	282	OE2	GLU A	107	34.608	5.654	-2.263	1.00	36.00	A
35	ATOM	283	C	GLU A	107	40.053	5.678	-1.410	1.00	18.93	A
	ATOM	284	0	GLU A	107	39.891	5.427	-0.220	1.00	19.21	A
	ATOM	285	N	TYR A	108	40.988	6.507	-1.852	1.00	16.70	A
	ATOM	286	CA	TYR A	108	41.883	7.209	-0.942	1.00	15.86	A
	ATOM	287	CB	TYR A	108	43.325	6.728	-1.104	1.00	15.30	A
40	MOTA	288	CG	TYR A	108	43.593	5.328	-0.612	1.00	16.33	A
	MOTA	289	CD1	TYR A	108	43.765	5.066	0.746	1.00	16.36	A
	ATOM	290	CE1	TYR A	108	44.046	3.769	1.201	1.00	18.48	A
	ATOM	291	CD2	TYR A	108	43.701	4.268	-1.511	1.00	13.25	A
	ATOM	292	CE2	TYR A	108	43.980	2.981	-1.075	1.00	17.28	A
45	ATOM	293	CZ	TYR A	108	44.152	2.736	0.276	1.00	19.17	A
	MOTA	294	OH	TYR A	108	44.440	1.461	0.688	1.00	19.38	A
	ATOM	295	С	TYR A	108	41.850	8.687	-1.292	1.00	16.80	A
	ATOM	296	0	TYR A	108	41.560	9.058	-2.431	1.00	15.22	A
	ATOM	297	N	ALA A	109	42.132	9.528	-0.306	1.00	14.61	A
50	MOTA	298	CA	ALA A	109	42.207	10.957	-0.539	1.00	14.30	A
	ATOM	299	CB	ALA A	109	41.671	11.726	0.661	1.00	14.78	A
	ATOM	300	C	ALA A	109	43.713	11.136	-0.667	1.00	16.79	A
	MOTA	301	0	ALA A	109	44.450	10.983	0.317	1.00	16.52	A
	MOTA	302	N	ILE A	110	44.182	11.410	-1.881	1.00	14.80	A
55	MOTA	303	CA	ILE A	110	45.609	11.574	-2.093	1.00	15.80	A
	ATOM	304	CB	ILE A	110	46.065	10.863	-3.396	1.00	16.85	A
	ATOM	305		ILE A		47.550	11.098	-3.632	1.00	16.80	A
	ATOM	306		ILE A		45.774	9.358	-3.284	1.00		A
	ATOM	307	CD1	ILE A	110	46.308	8.513	-4.437	1.00	16.07	A

	3.0001	308		TT D		110	46 004	12 045	0 100	1 00	17 70	
	MOTA		C	ILE			46.004	13.045	-2.129		17.78	A
	ATOM	309	0	ILE			45.534	13.813	-2.976		16.24	A
	ATOM	310	N	LYS	Α	111	46.846	13.435	-1.177	1.00	16.15	A
	ATOM	311	CA	LYS	Α	111	47.326	14.808	-1.100	1.00	17.20	A
5	ATOM	312	CB	LYS	A	111	47.700	15.176	0.344		17.41	A
	ATOM	313	CG	LYS			48.350	16.547	0.464		20.71	A
	ATOM	314	CD	LYS			48.585	16.971	1.910		24.25	A
	MOTA	315	CE	LYS			47.288	17.381	2.598		29.46	A
	MOTA	316	NZ	LYS			47.516	17.866	4.000		30.50	A
10	MOTA	317	С	LYS			48.551	14.890	-1.994		16.41	A
	ATOM	318	0	LYS	Α	111	49.509	14.137	-1.813	1.00	18.20	A.
	ATOM	319	N	ILE	Α	112	48.509	15.798	-2.963	1.00	15.87	A.
	ATOM	320	CA	ILE	Α	112	49.606	15.967	-3.907	1.00	17.28	A
	ATOM	321	CB	ILE	А	112	49.079	15.911	-5.358	1.00	16.43	A
15	ATOM	322		ILE			50.235	15.998	-6.341		15.12	A
	ATOM	323		ILE			48.293	14.609	-5.565		16.82	A
	ATOM	324		ILE			47.580	14.511	-6.904		18.47	A
	MOTA	325	С	ILE			50.307	17.301	-3.663		19.03	A
	MOTA	326	0	ILE			49.669	18.350	-3.635		19.15	A
20	ATOM	327	N	LEU			51.622	17.245	-3.472		20.22	A
	ATOM	328	CA	LEU	Α	113	52.416	18.442	-3.214		22.36	A
	MOTA	329	CB	LEU	Α	113	52.995	18.397	-1.794	1.00	22.13	A.
	ATOM	330	CG	LEU	Α	113	52.042	18.063	-0.646	1.00	22.46	A
	ATOM	331	CD1	LEU	А	113	51.866	16.557	-0.553	1.00	23.81	A
25	ATOM	332		LEU			52.603	18.595	0.660		23.68	A
20	ATOM	333	C	LEU			53.560	18.547	-4.215		23.37	A
	ATOM	334	o	LEU			54.300	17.586	-4.424		23.11	A
	MOTA	335	N	GLU			53.706	19.714	-4.834		23.88	A
	MOTA	336	CA	GLU			54.771	19.920	-5.806		26.00	A
30	ATOM	337	CB	GLU			54.435	21.111	-6.706		27.74	A
	ATOM	338	CG	GLU	Α	114	55.533	21.452	-7.696	1.00	35.07	A
	ATOM	339	CD	GLU	Α	114	55.220	22.696	-8.497	1.00	39.24	A.
	ATOM	340	OE1	GLU	Α	114	54.808	23.703	-7.885	1.00	41.45	A
	ATOM	341	OE2	GLU	А	114	55.395	22.670	-9.736	1.00	44.05	A
35	ATOM	342	С	GLU			56.087	20.163	-5.067		24.37	A.
00	ATOM	343	ŏ	GLU			56.186	21.071	-4.238		24.43	A
	ATOM	344	N	LYS			57.096	19.350	-5.360		24.10	A
											24.10	A
	ATOM	345	CA	LYS			58.376	19.493	-4.678			
40	MOTA	346	CB	LYS			59.339	18.373	-5.103		23.72	A
40	MOTA	347	CG	LYS			59.139	17.080	-4.308		23.09	A
	ATOM	348	CD	LYS			60.064	15.944	-4.743		21.92	A.
	ATOM	349	CE	LYS			59.691	15.400	-6.117		22.42	A
	ATOM	350	NZ	LYS	Α	115	60.447	14.150	-6.448	1.00	19.71	A.
	MOTA	351	C	LYS	Α	115	59.031	20.858	-4.868	1.00	26.87	A.
45	ATOM	352	0	LYS	Α	115	59.492	21.469	-3.903	1.00	26.17	A
	MOTA	353	N	ARG			59.058	21.348	-6.102		28.73	A.
	ATOM	354	CA	ARG			59.678	22.638	-6.380		29.66	A
	ATOM	355	CB	ARG	-	116	59.533	22.980	-7.868		31.29	AC1
50	MOTA	356	CG	ARG		116	60.047	24.361	-8.267		33.19	AC1
50	MOTA	357	CD	ARG		116	61.368	24.710	-7.590		35.13	AC1
	ATOM	358	NE	ARG		116	62.329	23.612	-7.618		36.42	AC1
	ATOM	359	CZ	ARG		116	63.510	23.648	-7.009	0.50	36.18	AC1
	ATOM	360	NH1	ARG		116	63.871	24.729	-6.332	0.50	36.12	AC1
	MOTA	361	NH2	ARG		116	64.324	22.602	-7.067	0.50	35.77	AC1
55	ATOM	362	С	ARG	А		59.097	23.761	-5.519		29.70	A
	ATOM	363	0	ARG			59.843	24.515	-4.889		29.16	A
	ATOM	364	N	HIS			57.773	23.862	-5.472		27.22	A
	ATOM	365	CA	HIS			57.126	24.903	-4.681		26.33	A
	MOTA	366	CB	HIS	А	11/	55.606	24.835	-4.848	1.00	28.41	A

	3.0001	2.67	00	*****		117	E4 001	0.0	4 050	1 00 31 00	
	MOTA	367	CG			117	54.881	26.005	-4.258	1.00 31.82	A
	ATOM	368	CD2	HIS	А	117	55.309	27.249	-3.935	1.00 33.19	A
	ATOM	369	ND1	HIS	Α	117	53.536	25.974	-3.961	1.00 34.30	A
	ATOM	370	CE1	HIS	Δ	117	53.165	27.148	-3.480	1.00 34.58	A
5											
	ATOM	371		HIS			54.222	27.940	-3.455	1.00 35.18	A
	MOTA	372	C	HIS			57.477	24.780	-3.202	1.00 26.22	A
	ATOM	373	0	HIS	А	117	57.737	25.776	-2.534	1.00 25.67	A
	ATOM	374	N	TLE	Δ	118	57.469	23.554	-2.689	1.00 24.94	A
	ATOM	375	CA			118	57.792	23.315	-1.285	1.00 23.94	A
10	MOTA	376	CB			118	57.711	21.812	-0.952	1.00 23.50	A
	ATOM	377	CG2	ILE	Α	118	58.374	21.533	0.389	1.00 23.76	A
	ATOM	378	CG1	ILE	А	118	56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379		ILE			56.066	19.858	-0.834	1.00 28.06	A
	ATOM	380	C			118	59.195	23.821	-0.958	1.00 23.78	A
15	MOTA	381	0			118	59.402	24.495	0.048	1.00 23.49	A
	ATOM	382	N	ILE	Α	119	60.153	23.489	-1.815	1.00 23.46	A
	ATOM	383	CA	ILE	А	119	61.534	23.913	-1.619	1.00 25.13	A
	ATOM	384	CB	TTF	70	119	62.467	23.250	-2.664	1.00 24.25	A
	ATOM	385		ILE			63.858	23.890	-2.617	1.00 22.47	A
20	MOTA	386		ILE			62.540	21.738	-2.395	1.00 25.05	A
	MOTA	387	CD1	ILE	Α	119	63.327	20.945	-3.439	1.00 24.62	A
	ATOM	388	C	ILE	Α	119	61.667	25.435	-1.705	1.00 25.96	A
	ATOM	389	0			119	62.330	26.051	-0.872	1.00 24.78	A
						120		26.039	-2.704		
	MOTA	390	N				61.028			1.00 27.67	A
25	MOTA	391	CA			120	61.100	27.489	-2.879	1.00 30.29	A
	MOTA	392	CB	LYS	Α	120	60.242	27.940	-4.060	1.00 32.34	A
	ATOM	393	CG	LYS	Α	120	60.674	27.407	-5.409	1.00 39.30	A
	ATOM	394	CD	LYS			59.765	27.950	-6.512	1.00 45.19	A
	ATOM	395	CE	LYS			58.294	27.636	-6.218	1.00 46.48	A
20											
30	MOTA	396	NZ			120	57.363	28.155	-7.252	1.00 46.49	A
	MOTA	397	C	LYS	Α	120	60.647	28.247	-1.638	1.00 30.89	A
	ATOM	398	0	LYS	Α	120	61.303	29.198	-1.217	1.00 32.48	A
	ATOM	399	N	GLII	Δ	121	59.527	27.825	-1.055	1.00 29.82	A
	ATOM	400	CA			121	58.986	28.488	0.128	1.00 30.33	A
2.5											
35	MOTA	401	CB			121	57.455	28.416	0.117	1.00 33.04	A
	ATOM	402	CG			121	56.794	29.021	-1.120	1.00 36.45	A
	ATOM	403	CD	GLU	Α	121	57.221	30.456	-1.373	1.00 39.88	A
	MOTA	404	OE1	GLU	А	121	57.200	31.264	-0.420	1.00 40.53	A
	ATOM	405		GLU			57.573	30.778	-2.529	1.00 43.24	A
40											
40	MOTA	406	С	GLU			59.511	27.930	1.451	1.00 30.37	A
	ATOM	407	0			121	58.946	28.204	2.513	1.00 31.24	A
	MOTA	408	N	ASN	Α	122	60.588	27.151	1.390	1.00 29.03	A
	ATOM	409	CA	ASN	Α	122	61.183	26.573	2.594	1.00 28.46	A
	ATOM	410	CB	ASN	Δ	122	61.836	27.673	3.436	1.00 31.28	A
45	ATOM	411	CG	ASN			62.945	28.395	2.698	1.00 34.12	A
43											
	MOTA	412		ASN			62.697	29.143	1.754	1.00 35.57	A
	ATOM	413	ND2	ASN	Α	122	64.181	28.169	3.127	1.00 35.73	A
	ATOM	414	C	ASN	Α	122	60.157	25.835	3.456	1.00 26.89	A
	ATOM	415	0	ASN			60.085	26.055	4.663	1.00 27.23	A
50	ATOM	416	N			123	59.375	24.955	2.842	1.00 23.99	A
50											
	MOTA	417	CA	LYS			58.358	24.210	3.574	1.00 22.43	A
	MOTA	418	CB	LYS	Α	123	57.031	24.248	2.810	1.00 21.97	A
	ATOM	419	CG	LYS	Α	123	56.475	25.645	2.599	1.00 25.68	A
	ATOM	420	CD			123	56.253	26.354	3.927	1.00 27.54	A
55	ATOM	421	CE	LYS				27.796	3.716	1.00 31.30	A
55							55.822				
	MOTA	422	NZ	LYS			55.756	28.540	5.004	1.00 33.21	A
	ATOM	423	C	LYS	Α	123	58.748	22.759	3.821	1.00 22.20	A
	MOTA	424	0	LYS	Α	123	57.924	21.960	4.264	1.00 22.50	A
	ATOM	425	N			124	59.997	22.412	3.535	1.00 20.59	A

	ATOM	426	CA	VAL	А	124	60.439	21.039	3.730	1.00	20.25	A
	ATOM	427	CB			124	61.922	20.850	3.328	1.00		A
	ATOM	428		VAL			62.346	19.407	3.573	1.00		A
	ATOM	429		VAL			62.104	21.195	1.853	1.00		A
5	ATOM	430	C			124	60.236	20.561	5.163	1.00		A
,	ATOM	431	Ö	VAL			59.841	19.418	5.385	1.00		A
	ATOM	431	N			125	60.513	21.422		1.00		A A
									6.159			
	MOTA	433	CD			125	61.178	22.738	6.118	1.00		A
	ATOM	434	CA			125	60.318	20.979	7.544	1.00		A
10	MOTA	435	CB			125	60.793	22.180	8.363	1.00		A
	MOTA	436	CG			125	61.839	22.805	7.479	1.00		A
	ATOM	437	C			125	58.848	20.642	7.824	1.00		A
	MOTA	438	0	PRO	Α	125	58.544	19.700	8.550	1.00		A
	ATOM	439	N	TYR	Α	126	57.947	21.418	7.235	1.00	18.98	A
15	MOTA	440	CA	TYR	Α	126	56.516	21.220	7.435	1.00	21.97	A
	ATOM	441	CB	TYR	Α	126	55.752	22.448	6.933	1.00	25.17	A
	ATOM	442	CG	TYR	Α	126	56.040	23.690	7.748	1.00	30.98	A
	ATOM	443	CD1	TYR	Α	126	55.438	23.886	8.991	1.00	33.95	A
	ATOM	444	CE1	TYR	Α	126	55.721	25.015	9.763	1.00	36.60	A
20	ATOM	445	CD2	TYR			56.938	24.657	7.292	1.00		A
	ATOM	446	CE2	TYR			57.231	25.792	8.058	1.00		A
	ATOM	447	CZ			126	56.618	25.962	9.291	1.00		A
	ATOM	448	OH			126	56.903	27.073	10.052	1.00		A
	ATOM	449	C			126	55.990	19.956	6.762	1.00		A
25	ATOM	450	o			126	55.265	19.175	7.383	1.00		A
23	ATOM	451	N			127	56.354	19.746	5.501	1.00		A
	ATOM	452							4.790	1.00		
			CA			127	55.892	18.562				A
	ATOM	453	CB			127	56.308	18.596	3.308	1.00		A
	MOTA	454		VAL			55.786	17.350	2.600	1.00		A
30	MOTA	455		VAL			55.751	19.850	2.641	1.00		A
	ATOM	456	C			127	56.459	17.306	5.448	1.00		A
	ATOM	457	0			127	55.769	16.298	5.583	1.00		A
	ATOM	458	N			128	57.716	17.381	5.869	1.00		A
	ATOM	459	CA			128	58.375	16.260	6.530	1.00		A
35	MOTA	460	CB	THR	Α	128	59.861	16.586	6.805	1.00	18.01	A
	ATOM	461	OG1	THR	Α	128	60.537	16.804	5.559	1.00	21.14	A
	MOTA	462	CG2	THR	A	128	60.536	15.446	7.545	1.00	17.95	A
	MOTA	463	C	THR	Α	128	57.676	15.941	7.856	1.00	19.49	A
	MOTA	464	0	THR	Α	128	57.438	14.776	8.179	1.00	18.76	A
40	ATOM	465	N	ARG	Α	129	57.345	16.981	8.619	1.00	19.60	A
	ATOM	466	CA	ARG	А	129	56.673	16.804	9.904	1.00	20.12	A
	ATOM	467	СВ	ARG	А	129	56.534	18.144	10.621	1.00	21.33	A
	ATOM	468	CG	ARG			55.948	18.029	12.023	1.00		A
	ATOM	469	CD	ARG			55.721	19.404	12.597	1.00		A
45	ATOM	470	NE	ARG			56.940	20.205	12.560	1.00		A
.5	ATOM	471	CZ			129	56.962	21.524	12.391	1.00		A
	ATOM	472		ARG			55.828	22.197	12.239	1.00		A
	ATOM	473		ARG			58.119	22.170	12.233	1.00		A
		474	C	ARG			55.288	16.186	9.729	1.00		
50	ATOM											A
30	ATOM	475	0	ARG			54.891	15.305	10.496	1.00		A
	ATOM	476	N			130	54.553	16.654	8.724	1.00		A
	MOTA	477	CA	GLU			53.222	16.125	8.454	1.00		A
	MOTA	478	CB	GLU			52.638	16.749	7.183	1.00		A
	MOTA	479	CG	GLU			51.350	16.087	6.708	1.00		A
55	MOTA	480	CD			130	50.581	16.933	5.707	1.00		A
	MOTA	481		GLU			51.216	17.528	4.814	1.00		A
	MOTA	482	OE2				49.339	16.996	5.807	1.00		A
	ATOM	483	C	GLU	Α	130	53.301	14.615	8.295	1.00	19.81	A
	ATOM	484	0	GLU	Α	130	52.553	13.875	8.935	1.00	18.37	A

	ATOM	485	N	ARG	Α	131	54.219	14.162	7.447	1.00	20.41	A
	ATOM	486	CA	ARG	Α	131	54.397	12.735	7.202	1.00	22.45	A
	MOTA	487	CB	ARG	Α	131	55.442	12.511	6.098	1.00	25.16	A
	ATOM	488	CG	ARG	Α	131	55.742	11.043	5.840	1.00	28.75	A
5	ATOM	489	CD	ARG	Α	131	56.736	10.837	4.708	1.00	33.75	A
	MOTA	490	NE	ARG	Α	131	57.020	9.415	4.520	1.00	40.07	A
	ATOM	491	CZ	ARG	Α	131	57.756	8.915	3.532	1.00	43.07	A
	MOTA	492	NH1	ARG	Α	131	58.293	9.721	2.625	1.00	44.91	A
	ATOM	493	NH2	ARG	Α	131	57.955	7.606	3.449	1.00	44.45	A
10	ATOM	494	C	ARG	Α	131	54.820	11.982	8.466	1.00	23.24	A
	ATOM	495	0	ARG	Α	131	54.241	10.948	8.804	1.00	23.86	A
	ATOM	496	N	ASP	Α	132	55.831	12.497	9.160	1.00	21.99	A
	ATOM	497	CA	ASP	Α	132	56.318	11.850	10.370	1.00	22.04	A
	ATOM	498	CB	ASP	Α	132	57.570	12.564	10.888	1.00	23.72	A
15	MOTA	499	CG	ASP	Α	132	58.750	12.442	9.932	1.00	27.77	A
	ATOM	500	OD1	ASP	Α	132	58.681	11.620	8.989	1.00	27.34	A
	ATOM	501	OD2	ASP	Α	132	59.753	13.163	10.128	1.00	28.70	A
	MOTA	502	C	ASP	Α	132	55.258	11.772	11.474	1.00	21.69	A
	MOTA	503	0	ASP	Α	132	55.077	10.723	12.092	1.00	22.75	A
20	MOTA	504	N	VAL	Α	133	54.551	12.868	11.725	1.00	19.54	A
	MOTA	505	CA			133	53.525	12.843	12.759	1.00	18.52	A
	MOTA	506	CB	VAL	Α	133	52.908	14.244	12.990	1.00	19.26	A
	MOTA	507	CG1	VAL	Α	133	51.708	14.135	13.918	1.00	18.79	A
	MOTA	508	CG2	VAL	Α	133	53.953	15.180	13.604	1.00	18.80	A
25	MOTA	509	C	VAL	Α	133	52.419	11.854	12.398	1.00	19.46	A
	ATOM	510	0	VAL	Α	133	52.073	10.991	13.200	1.00	19.94	A
	ATOM	511	N	MET			51.878	11.957	11.187		19.15	A
	MOTA	512	CA	MET			50.807	11.052	10.792		21.25	A
	MOTA	513	CB	MET	Α	134	50.309	11.381	9.383		17.34	A
30	MOTA	514	CG	MET			49.615	12.730	9.302		20.00	A
	ATOM	515	SD	MET			48.643	12.952	7.798		24.21	A
	ATOM	516	CE	MET			47.033	12.434	8.400		23.20	A
	MOTA	517	С	MET			51.203	9.582	10.881		22.43	A
	MOTA	518	0	MET			50.384	8.741	11.249		23.82	A
35	ATOM	519	N	SER			52.454	9.273	10.556		23.09	A
	MOTA	520	CA	SER			52.939	7.895	10.615		26.13	A
	MOTA	521	CB	SER			54.356	7.798	10.039		26.17	A
	MOTA	522	OG	SER			54.383	8.177	8.673		31.91	A
	MOTA	523	С			135	52.957	7.358	12.045		26.58	A
40	MOTA	524	0	SER			52.926	6.148	12.261		26.42	A
	MOTA	525	N			136	53.014	8.261	13.018		25.65	A
	ATOM	526	CA	ARG			53.056	7.870	14.425		27.47	A
	ATOM	527	CB	ARG			53.823	8.914	15.238		27.97	A
	MOTA	528	CG	ARG			55.283	9.082	14.857		32.00	A
45	MOTA	529	CD	ARG			55.904	10.218	15.664		33.03	A
	ATOM	530	NE	ARG			55.602	10.073	17.084		36.11	A
	ATOM	531	CZ	ARG			55.867	10.990	18.007		39.74	A
	ATOM	532		ARG			56.449	12.132	17.661		40.55	A
50	ATOM	533		ARG			55.540	10.769	19.276		36.72	A
50	ATOM	534	C	ARG			51.667	7.709	15.036		26.38	A
	MOTA	535	0	ARG			51.516	7.121	16.106		27.06	A
	MOTA	536	N	LEU			50.655	8.235	14.360		24.77	A
	ATOM	537	CA	LEU			49.294	8.162	14.870		24.70	A
55	ATOM	538	CB	LEU			48.483	9.363	14.371		24.52	A
23	ATOM	539	CG CD1	LEU			49.050	10.760	14.662		26.67	A
	MOTA	540		LEU			48.075	11.813	14.141		27.25	A
	MOTA	541		LEU			49.279	10.945	16.155		27.09	A
	ATOM	542	C	LEU			48.592	6.868	14.473		25.20	A
	ATOM	543	0	LEU	Α	13/	48.619	6.469	13.309	1.00	∠5.99	A

	ATOM	544	N	ASP	А	138	47.971	6.218	15.451	1.00 21.89	A
	ATOM	545	CA			138	47.239	4.977	15.219	1.00 21.35	A
	ATOM	546	CB	ASP			48.124	3.761	15.523	1.00 22.14	A
	ATOM	547	CG	ASP			47.432	2.448	15.201	1.00 24.90	A
5	ATOM	548		ASP			46.631	2.423	14.241	1.00 24.78	A
-	ATOM	549		ASP			47.691	1.443	15.897	1.00 25.39	A
	ATOM	550	C	ASP			46.031	4.991	16.138	1.00 20.47	A
	ATOM	551	0	ASP			45.967	4.248	17.118	1.00 19.06	A
10	ATOM	552	N	HIS			45.075	5.852	15.810	1.00 18.27	A
10	MOTA	553	CA	HIS			43.869	6.016	16.606	1.00 18.21	A
	MOTA	554	CB	HIS			44.096	7.157	17.612	1.00 15.84	A
	ATOM	555	CG	HIS			42.985	7.332	18.600	1.00 15.24	A
	MOTA	556		HIS			42.884	6.964	19.900	1.00 13.97	A
	MOTA	557		HIS			41.791	7.943	18.280	1.00 14.74	A
15	ATOM	558	CE1	HIS	Α	139	41.002	7.944	19.341	1.00 14.19	A
	MOTA	559	NE2	HIS	Α	139	41.641	7.356	20.336	1.00 14.15	A.
	MOTA	560	C	HIS	Α	139	42.715	6.330	15.654	1.00 18.50	A
	ATOM	561	0	HIS	Α	139	42.879	7.080	14.693	1.00 20.80	A
	ATOM	562	N	PRO	Α	140	41.527	5.767	15.913	1.00 18.32	A
20	ATOM	563	CD	PRO	Α	140	41.143	4.984	17.100	1.00 16.71	A
	ATOM	564	CA	PRO	Α	140	40.367	6.001	15.048	1.00 17.43	A
	ATOM	565	CB	PRO	А	140	39.273	5.157	15.704	1.00 16.64	A
	ATOM	566	CG			140	39.643	5.204	17.152	1.00 18.43	A
	ATOM	567	C			140	39.914	7.441	14.803	1.00 18.77	A
25	ATOM	568	ō			140	39.207	7.695	13.831	1.00 19.88	A
	ATOM	569	N			141	40.301	8.381	15.664	1.00 17.14	A
	ATOM	570	CA			141	39.874	9.767	15.477	1.00 16.42	A
	ATOM	571	CB			141	39.568	10.422	16.836	1.00 14.60	A
	ATOM	572	CG			141	38.386	9.817	17.556	1.00 15.26	A
30	ATOM	573		PHE			37.335	9.234	16.842	1.00 14.78	A
30	ATOM	574	CD1	PHE			38.297	9.234	18.942	1.00 14.78	
											A
	MOTA	575		PHE			36.215	8.727	17.502	1.00 16.94	A
	MOTA	576		PHE			37.178	9.375	19.615	1.00 15.75	A
	MOTA	577	CZ			141	36.135	8.799	18.893	1.00 16.89	A
35	MOTA	578	C			141	40.857	10.641	14.694	1.00 16.15	A
	MOTA	579	0			141	40.799	11.871	14.761	1.00 17.35	A
	MOTA	580	N			142	41.748	10.011	13.941	1.00 15.88	A
	ATOM	581	CA			142	42.727	10.756	13.154	1.00 17.89	A
	MOTA	582	CB			142	44.115	10.645	13.793	1.00 17.57	A
40	MOTA	583	CG	PHE	Α	142	44.240	11.371	15.103	1.00 18.74	A
	MOTA	584	CD1	PHE	Α	142	44.559	12.726	15.135	1.00 17.77	A
	MOTA	585	CD2	PHE	Α	142	43.997	10.711	16.304	1.00 18.74	A
	MOTA	586	CE1	PHE	Α	142	44.632	13.417	16.347	1.00 15.77	A
	ATOM	587	CE2	PHE	Α	142	44.065	11.393	17.522	1.00 17.56	A
45	ATOM	588	CZ	PHE	Α	142	44.383	12.747	17.542	1.00 17.14	A
	MOTA	589	C	PHE	Α	142	42.793	10.231	11.729	1.00 19.12	A
	ATOM	590	0	PHE	Α	142	42.659	9.030	11.504	1.00 20.01	A
	ATOM	591	N			143	42.978	11.135	10.769	1.00 18.72	A
	ATOM	592	CA			143	43.102	10.735	9.371	1.00 18.52	A
50	ATOM	593	CB			143	43.294	11.961	8.440	1.00 20.66	A
	ATOM	594		VAL			43.843	11.521	7.080	1.00 21.29	A
	ATOM	595		VAL			41.958	12.673	8.252	1.00 22.97	A
	ATOM	596	C			143	44.342	9.865	9.330	1.00 18.68	A
	ATOM	597	o	VAL			45.355	10.199	9.943	1.00 18.42	A
55	ATOM	598	N			144	44.259	8.745	8.623	1.00 18.42	A
55	ATOM	599	CA			144		7.824	8.535	1.00 18.30	
							45.384	6.373			A
	ATOM	600	CB			144	44.889		8.608	1.00 22.27	A
	ATOM	601	CG			144	46.017	5.340	8.557	1.00 29.72	A
	MOTA	602	CD	LYS	Α	144	45.491	3.912	8.674	1.00 34.16	A

	ATOM	603	CE	LYS	144	46.631	2.896	8.577	1.00	37.67	A
	ATOM	604	NZ	LYS	144	46.138	1.484	8.629	1.00	39.02	A
	ATOM	605	C		144	46.192	8.002	7.261		18.53	A
	ATOM	606	ō		144	45.643	8.314	6.200		18.18	A
5	ATOM	607	N		145	47.502	7.816	7.385		16.79	A
	ATOM	608	CA		145	48.411	7.900	6.251		17.45	A
	ATOM	609	CB	LEU	145	49.686	8.653	6.641		18.82	AC1
	ATOM	610	CG	LEU	145	50.734	8.902	5.549		20.23	AC1
	ATOM	611		LEU	145	51.836	9.799	6.093		18.83	AC1
10					145		7.581	5.069			AC1
10	MOTA	612		LEU		51.317				19.79	
	MOTA	613	С		145	48.739	6.450	5.907		19.19	A
	MOTA	614	0		145	49.451	5.772	6.659		17.36	A
	MOTA	615	N		146	48.215	5.972	4.782		17.28	A
	ATOM	616	CA		146	48.444	4.593	4.358		17.57	A
15	MOTA	617	CB		146	47.288	4.098	3.486		17.74	A
	MOTA	618	CG		146	45.981	3.926	4.214		17.50	A
	MOTA	619		TYR 2		45.099	4.995	4.377		16.50	A
	ATOM	620		TYR 2		43.881	4.827	5.039	1.00	17.10	A
	MOTA	621	CD2	TYR 2	146	45.620	2.686	4.735	1.00	18.28	A
20	MOTA	622	CE2	TYR 2	146	44.411	2.506	5.399	1.00	19.84	A
	ATOM	623	CZ	TYR 2	A 146	43.547	3.576	5.544	1.00	17.53	A
	ATOM	624	OH	TYR 2	A 146	42.342	3.376	6.169	1.00	20.67	A
	ATOM	625	C	TYR 2	146	49.735	4.376	3.582	1.00	18.72	A
	ATOM	626	0	TYR 2	146	50.382	3.338	3.715	1.00	19.51	A
25	ATOM	627	N		147	50.110	5.350	2.765		18.09	A
	ATOM	628	CA		147	51.307	5.203	1.952		17.20	A
	ATOM	629	CB		147	51.007	4.258	0.783		16.77	A
	ATOM	630	CG		147	49.835	4.699	-0.070		17.75	A
	ATOM	631		PHE 2		49.967	5.752	-0.975		16.58	A
30	ATOM	632		PHE 2		48.595	4.075	0.053		18.07	A
50	ATOM	633		PHE 2		48.886	6.178	-1.742		19.62	A
	ATOM	634		PHE		47.503	4.492	-0.710		18.56	A
	ATOM	635	CZ		A 147		5.546	-1.610		19.27	A
						47.647					
2.5	ATOM	636	С		A 147	51.768	6.533	1.395		17.13	A
35	MOTA	637	0		147	51.045	7.528	1.452		14.43	A
	MOTA	638	N		148	52.981	6.534	0.854		17.12	A
	MOTA	639	CA		148	53.541	7.718	0.232		17.96	A
	MOTA	640	CB		148	54.449	8.531	1.197		21.51	A
	MOTA	641		THR 3		55.605	7.760	1.537		18.83	A
40	MOTA	642		THR 2		53.700	8.897	2.472		19.60	A
	MOTA	643	C		148	54.386	7.262	-0.946		20.31	A
	MOTA	644	0		148	54.860	6.124	-0.991		18.94	A
	ATOM	645	N		A 149	54.543	8.149	-1.916	1.00	19.16	A
	MOTA	646	CA	PHE 2	149	55.368	7.877	-3.073	1.00	18.01	A
45	ATOM	647	CB	PHE 2	A 149	54.748	6.801	-3.989	1.00	17.23	A
	ATOM	648	CG	PHE 2	149	53.389	7.144	-4.544	1.00	16.88	A
	ATOM	649	CD1	PHE 2	A 149	53.262	7.888	-5.712	1.00	18.58	A
	ATOM	650		PHE 2		52.235	6.668	-3.927		17.31	A
	ATOM	651		PHE		52.007	8.149	-6.267		19.26	A
50	ATOM	652		PHE		50.972	6.923	-4.470		19.17	A
	ATOM	653	CZ		149	50.858	7.663	-5.642		19.60	A
	ATOM	654	C		149	55.542	9.205	-3.774		20.85	A
	ATOM	655	0		A 149	54.934	10.200	-3.376		19.76	A
	ATOM	656	N		4 149 4 150	56.398	9.241	-4.782		19.79	A
55	ATOM	657	CA		4 150 4 150	56.636	10.481	-5.497		24.03	A A
23											
	MOTA	658	CB		150	57.659	11.347	-4.739		24.45	A
	MOTA	659	CG		150	58.986	10.645	-4.414		26.28	A
	MOTA	660	CD		150	59.988	11.558	-3.692		29.02	A
	ATOM	661	OE1	GLN 2	A 150	60.693	12.353	-4.321	1.00	27.05	A

	ATOM	662	arm o	GLN		150	60.042	11.449	-2.365	1.00 26.	12 2
	ATOM	663	C	GLN	А	150	57.160	10.203	-6.885	1.00 23.	
	ATOM	664	0	GLN	Α	150	57.673	9.118	-7.158	1.00 24.7	79 A
	ATOM	665	N	ASP	Δ	151	56.987	11.171	-7.774	1.00 25.4	38 A
5											
3	ATOM	666	CA	ASP			57.527	11.047	-9.117	1.00 26.	
	MOTA	667	CB	ASP	Α	151	56.437	11.126	-10.199	1.00 24.	54 A
	ATOM	668	CG	ASP	Α	151	55.544	12.336	-10.064	1.00 24.	95 A
	ATOM	669	OD1	ASP	75	151	56.005	13.379	-9.561	1.00 22.	
	MOTA	670		ASP			54.369		-10.490	1.00 25.	
10	MOTA	671	C	ASP			58.515	12.203	-9.220	1.00 28.	
	ATOM	672	0	ASP	А	151	58.890	12.780	-8.194	1.00 27.1	33 A
	ATOM	673	N	ASP	Δ	152	58.934	12.560	-10.426	1.00 29.2	
	ATOM	674	CA	ASP			59.907		-10.562	1.00 31.4	
	ATOM	675	CB	ASP			60.325		-12.026	1.00 33.	
15	MOTA	676	CG	ASP	Α	152	61.033	12.564	-12.557	1.00 38.8	38 A
	ATOM	677	OD1	ASP	Α	152	61.817	11.959	-11.791	1.00 39.0	67 A
	ATOM	678		ASP			60.817		-13.738	1.00 41.	
	MOTA	679	C	ASP			59.487		-10.013	1.00 30.	
	MOTA	680	0	ASP	Α	152	60.316	15.735	-9.482	1.00 31.	69 A
20	ATOM	681	N	GLU	Α	153	58.207	15.322	-10.107	1.00 29.	44 A
	ATOM	682	CA	GLU	А	153	57.767	16.632	-9.646	1.00 28.	69 A
	ATOM	683	CB	GLU			56.984		-10.766	1.00 32.	
	ATOM	684	CG	GLU			57.451		-12.183	1.00 40.	
	ATOM	685	CD	GLU	Α	153	56.920	15.643	-12.675	1.00 45.	78 A
25	ATOM	686	OE1	GLU	Α	153	55.682	15.482	-12.760	1.00 48.	91 A
	ATOM	687	OE2	GLU	А	153	57.736	14.747	-12.979	1.00 48.	95 A
	ATOM	688	c	GLU			56.929	16.683	-8.372	1.00 26.	
	MOTA	689	0	GLU			56.947	17.688	-7.660	1.00 25.0	
	ATOM	690	N	LYS	Α	154	56.205	15.610	-8.069	1.00 22.	39 A
30	ATOM	691	CA	LYS	Α	154	55.318	15.631	-6.912	1.00 21.	43 A
	MOTA	692	CB	LYS			53.861	15.628	-7.398	1.00 20.	
	ATOM	693	CG	LYS			53.505	16.716	-8.403	1.00 21.	
	MOTA	694	CD	LYS			52.211	16.375	-9.146	1.00 19.	
	MOTA	695	CE	LYS	Α	154	51.775	17.503	-10.077	1.00 20.0	04 A
35	ATOM	696	NZ	LYS	Α	154	50.631	17.094	-10.951	1.00 19.5	97 A
	ATOM	697	С	LYS			55.458	14.522	-5.881	1.00 20.	
	MOTA	698	0	LYS			55.949	13.426	-6.173	1.00 21.	
	MOTA	699	N	LEU	A	155	54.985	14.832	-4.676	1.00 19.	69 A
	ATOM	700	CA	LEU	A	155	54.950	13.900	-3.553	1.00 19.3	10 A
40	ATOM	701	CB	LEU	А	155	55.362	14.588	-2.252	1.00 19.	65 A
	ATOM	702	CG	LEU			56.740	15.234	-2.129	1.00 21.3	
	MOTA	703		LEU			56.848	15.918	-0.770	1.00 23.	
	ATOM	704	CD2	LEU			57.816	14.174	-2.277	1.00 23.0	
	ATOM	705	C	LEU	A	155	53.478	13.507	-3.427	1.00 18.8	37 A
45	ATOM	706	0	LEU	А	155	52.600	14.348	-3.620	1.00 18.	61 A
	ATOM	707	N	TYR			53.209	12.249	-3.091	1.00 15.0	
	ATOM	708	CA	TYR			51.834	11.783	-2.934	1.00 16.2	
	MOTA	709	CB	TYR	Α	156	51.470	10.769	-4.029	1.00 14.3	20 A
	ATOM	710	CG	TYR	А	156	51.603	11.273	-5.449	1.00 17.3	29 A
50	ATOM	711		TYR			52.857	11.429	-6.045	1.00 16.	
50	ATOM	712	CE1	TYR			52.978	11.884	-7.360	1.00 18.	
	ATOM	713	CD2	TYR			50.474	11.588	-6.202	1.00 16.	
	MOTA	714	CE2	TYR	Α	156	50.583	12.048	-7.512	1.00 16.3	31 A
	MOTA	715	CZ	TYR	Α	156	51.835	12.192	-8.083	1.00 18.3	17 A
55	ATOM	716	OH	TYR			51.941	12.651	-9.371	1.00 17.	
22											
	MOTA	717	С	TYR			51.657	11.108	-1.572	1.00 16.	
	ATOM	718	0	TYR			52.412	10.197	-1.235	1.00 16.3	
	ATOM	719	N	PHE	Α	157	50.678	11.568	-0.792	1.00 15.	47 A
	ATOM	720	CA	PHE	Α	157	50.385	10.966	0.508	1.00 16.	66 A

	ATOM	721	CB	PHE	A	157	50.324	12.014	1.629	1.00 16	. 91	Α
	ATOM	722	CG			157	51.631	12.708	1.907	1.00 18		A
	ATOM	723	CD1	PHE	Α	157	52.821	12.261	1.340	1.00 20).31	Α
	ATOM	724	CD2	PHE	Α	157	51.664	13.829	2.732	1.00 21	.12	Α
5	ATOM	725	CE1				54.025	12.926	1.585	1.00 22		А
,												
	MOTA	726	CE2				52.865	14.500	2.982	1.00 22		A
	ATOM	727	CZ	PHE	Α	157	54.045	14.045	2.405	1.00 21	27	A
	ATOM	728	С	PHE	75	157	49.016	10.308	0.404	1.00 16	5.2	Α
	ATOM	729	0	PHE			48.029	10.979	0.110	1.00 17		А
10	ATOM	730	N	GLY	Α	158	48.953	9.002	0.644	1.00 15	5.97	A
	ATOM	731	CA	GLY	Z.	158	47.684	8.299	0.572	1.00 16	1.3	Α
	ATOM	732	С	GLY			47.000	8.383	1.920	1.00 14		Α
	ATOM	733	0	GLY	Α	158	47.445	7.756	2.879	1.00 16	.28	A
	ATOM	734	N	LEU	Δ	159	45.915	9.145	1.989	1.00 13	50	Α
15			CA	LEU			45.191	9.340	3.241	1.00 15		
13	MOTA	735										A
	ATOM	736	CB	LEU	Α	159	45.031	10.835	3.517	1.00 14	.20	Α
	ATOM	737	CG	LEU	А	159	46.270	11.726	3.385	1.00 19	.00	Α
	ATOM	738		LEU			45.847	13.188	3.477	1.00 17		A
	MOTA	739	CD2	LEU	А	159	47.275	11.390	4.471	1.00 14	.71	Α
20	ATOM	740	C	LEU	Α	159	43.809	8.716	3.232	1.00 15	5.53	Α
	ATOM	741	o	LEU			43.232	8.472	2.177	1.00 16		A
	ATOM	742	N	SER			43.268	8.469	4.418	1.00 15		Α
	ATOM	743	CA	SER	Α	160	41.932	7.917	4.498	1.00 19	.01	A
	ATOM	744	CB	SER	Δ	160	41.566	7.582	5.949	1.00 22	90	Α
25	ATOM	745	OG	SER			41.901	8.629	6.833	1.00 24		A
23												
	ATOM	746	C	SER	Α	160	40.987	8.968	3.924	1.00 20	0.43	Α
	ATOM	747	0	SER	А	160	41.213	10.173	4.062	1.00 19	.96	Α
	ATOM	748	N	TYR			39.945	8.508	3.250	1.00 19		Α
	MOTA	749	CA	TYR			38.975	9.406	2.644	1.00 20		Α
30	ATOM	750	CB	TYR	Α	161	38.471	8.785	1.332	1.00 20	.00	Α
	ATOM	751	CG	TYR			37.314	9.502	0.666	1.00 20		A
	ATOM	752		TYR			37.222	10.895	0.682	1.00 18		А
	ATOM	753	CE1	TYR	Α	161	36.180	11.557	0.029	1.00 22	.24	A
	ATOM	754	CD2	TYR	Δ	161	36.333	8.784	-0.020	1.00 20	1 53	Α
25												
35	ATOM	755		TYR			35.287	9.436	-0.678	1.00 24		A
	ATOM	756	CZ	TYR	Α	161	35.218	10.822	-0.648	1.00 22	.32	Α
	ATOM	757	OH	TYR	А	161	34.194	11.471	-1.298	1.00 23	1.03	Α
	ATOM	758	C	TYR			37.812	9.681	3.598	1.00 20		Α
	MOTA	759	0	TYR			36.959	8.819	3.810	1.00 19		Α
40	ATOM	760	N	ALA	Α	162	37.791	10.880	4.178	1.00 19	.92	Α
	ATOM	761	CA	ALA	А	162	36.721	11.271	5.099	1.00 21	. 07	Α
	ATOM	762	CB	ALA			37.187	12.419	6.002	1.00 19		A
	MOTA	763	C	ALA	Α	162	35.542	11.712	4.238	1.00 22		Α
	ATOM	764	0	ALA	Α	162	35.436	12.875	3.860	1.00 20).66	Α
45	ATOM	765	N	LYS			34.653	10.769	3.945	1.00 23		А
75												
	MOTA	766	CA	LYS			33.503	11.017	3.080	1.00 27		A
	ATOM	767	CB	LYS	Α	163	32.663	9.741	2.963	1.00 29	.68	Α
	ATOM	768	CG	LYS	Δ	163	33.455	8.524	2.515	1.00 37	67	Α
	MOTA	769	CD	LYS			32.556	7.310	2.321	1.00 42		Α
50	MOTA	770	CE	LYS	Α	163	33.373	6.034	2.185	1.00 44	.48	Α
	ATOM	771	NZ	LYS	А	163	34.143	5.735	3.430	1.00 44	. 88	Α
	ATOM	772	C	LYS			32.581	12.186	3.411	1.00 25		A
		773	0	LYS	Α	163	32.103	12.863	2.506	1.00 26	5.53	Α
	MOTA					1.64	00 000	10 441	4 600	1.00 24	- FD	_
		774	N	ASN	Α		32.321				.5/	А
55	MOTA	774		ASN			32.327	12.441	4.689			A.
55	ATOM ATOM	774 775	CA	ASN	Α	164	31.420	13.522	5.033	1.00 23	3.77	Α
55	MOTA MOTA MOTA	774 775 776	CA CB	ASN ASN	A A	164 164	31.420 30.610	13.522 13.129	5.033 6.265	1.00 23 1.00 25	3.77 5.02	A A
55	ATOM ATOM	774 775	CA	ASN	A A	164 164	31.420	13.522	5.033	1.00 23	3.77 5.02	Α
55	ATOM ATOM ATOM ATOM	774 775 776 777	CA CB CG	ASN ASN ASN	A A A	164 164 164	31.420 30.610 29.537	13.522 13.129 12.101	5.033 6.265 5.932	1.00 23 1.00 25 1.00 27	3.77 5.02 7.54	A A A
55	MOTA MOTA MOTA	774 775 776	CA CB CG OD1	ASN ASN	A A A	164 164 164 164	31.420 30.610	13.522 13.129	5.033 6.265	1.00 23 1.00 25	3.77 5.02 7.54 8.79	A A

	ATOM	780	C	ASN	Α	164	31.999	14.931	5.169	1.00 24.43	A
	ATOM	781	o	ASN			31.306	15.856	5.589	1.00 23.98	A
	ATOM	782	N	GLY			33.262	15.097	4.795	1.00 21.56	A
	ATOM	783	CA	GLY			33.873	16.414	4.836	1.00 24.39	A
5	ATOM	784	C	GLY			34.191	17.043	6.181	1.00 23.62	A
,	ATOM	785	Ö	GLY			34.380	16.352	7.177	1.00 23.02	A
	ATOM	786	N	GLU			34.234	18.373	6.186	1.00 23.22	A
	MOTA	787	CA	GLU			34.563	19.176	7.362	1.00 24.54	A
	MOTA	788	CB	GLU			35.055	20.558	6.913	1.00 25.04	A
10	MOTA	789	CG	GLU			36.419	20.569	6.229	1.00 26.48	A
	MOTA	790	CD	GLU			36.699	21.889	5.517	1.00 30.02	A
	ATOM	791		GLU			36.081	22.906	5.889	1.00 29.33	A
	MOTA	792	OE2	GLU	Α	166	37.544	21.916	4.596	1.00 30.48	A
	ATOM	793	C	GLU	Α	166	33.436	19.372	8.369	1.00 24.44	A
15	MOTA	794	0	GLU	Α	166	32.279	19.541	8.001	1.00 22.76	A
	ATOM	795	N	LEU	Α	167	33.791	19.370	9.649	1.00 22.95	A
	ATOM	796	CA	LEU	Α	167	32.813	19.581	10.707	1.00 22.26	A
	ATOM	797	CB	LEU	Α	167	33.497	19.481	12.073	1.00 22.32	A
	ATOM	798	CG	LEU			32.706	19.923	13.306	1.00 22.04	A
20	ATOM	799	CD1	LEU			31.454	19.074	13.463	1.00 19.66	A
	ATOM	800		LEU			33.597	19.805	14.537	1.00 21.17	A
	ATOM	801	C	LEU			32.193	20.971	10.529	1.00 23.49	A
	ATOM	802	ō	LEU			31.047	21.209	10.907	1.00 23.56	A
	ATOM	803	N	LEU			32.960	21.887	9.948	1.00 24.25	A
25	ATOM	804	CA	LEU			32.473	23.245	9.722	1.00 24.23	A
23											
	ATOM	805	CB	LEU			33.560	24.099	9.066	1.00 25.62	A
	MOTA	806	CG	LEU			33.198	25.546	8.707	1.00 27.34	A
	MOTA	807		LEU			32.718	26.296	9.946	1.00 26.42	A
	MOTA	808		LEU			34.418	26.238	8.119	1.00 26.74	A
30	MOTA	809	C	LEU			31.234	23.218	8.829	1.00 27.13	A
	MOTA	810	0	LEU			30.297	23.989	9.030	1.00 26.01	A
	ATOM	811	N	LYS			31.233	22.320	7.848	1.00 26.41	A
	MOTA	812	CA	LYS			30.106	22.210	6.934	1.00 27.70	A
	MOTA	813	CB	LYS			30.324	21.064	5.945	1.00 30.49	A
35	ATOM	814	CG	LYS	Α	169	29.151	20.854	4.993	1.00 32.47	A
	ATOM	815	CD	LYS	Α	169	29.407	19.728	3.998	1.00 35.98	A
	MOTA	816	CE	LYS	Α	169	29.462	18.372	4.683	1.00 38.53	A
	ATOM	817	NZ	LYS	Α	169	29.622	17.263	3.702	1.00 41.00	A
	ATOM	818	C	LYS	Α	169	28.801	21.985	7.682	1.00 28.12	A
40	ATOM	819	0	LYS	Α	169	27.785	22.608	7.371	1.00 28.08	A
	ATOM	820	N	TYR			28.826	21.094	8.668	1.00 26.53	A
	ATOM	821	CA	TYR			27.624	20.791	9.434	1.00 26.95	A
	ATOM	822	CB	TYR			27.810	19.476	10.193	1.00 25.03	A
	ATOM	823	CG	TYR			27.898	18.300	9.251	1.00 26.65	A
45	ATOM	824		TYR			26.745	17.661	8.790	1.00 28.27	A
75	ATOM	825		TYR			26.814	16.642	7.839	1.00 26.85	A
	ATOM	826		TYR			29.127	17.884	8.742	1.00 27.83	A
	ATOM	827		TYR			29.209	16.869	7.792	1.00 27.19	A
50	MOTA	828	CZ	TYR			28.049	16.254	7.343	1.00 30.02	A
50	MOTA	829	OH	TYR			28.130	15.268	6.382	1.00 29.23	A
	MOTA	830	С	TYR			27.229	21.918	10.376	1.00 27.59	A
	MOTA	831	0	TYR			26.045	22.122	10.642	1.00 29.25	A
	ATOM	832	N	ILE			28.208	22.660	10.882	1.00 28.16	A
	MOTA	833	CA	ILE			27.883	23.770	11.763	1.00 29.03	A
55	MOTA	834	CB	ILE			29.151	24.435	12.337	1.00 27.51	A
	MOTA	835		ILE			28.773	25.705	13.084	1.00 27.97	A
	ATOM	836	CG1	ILE	Α	171	29.872	23.458	13.272	1.00 26.70	A
	ATOM	837	CD1	ILE	Α	171	31.163	23.996	13.856	1.00 24.07	A
	ATOM	838	C	ILE	Α	171	27.094	24.796	10.944	1.00 31.41	A

	ATOM	839	0	ILE	А	171	- 2	26.088	25.335	11.407	1.00	31.69	A
	ATOM	840	N	ARG				27.546	25.047	9.719		33.21	A
	ATOM	841	CA	ARG				26.874	26.000	8.844		36.54	A
	ATOM	842	CB	ARG				27.734	26.314	7.616		37.73	A
5	ATOM	843	CG	ARG				29.057	27.011	7.912		41.65	A
-	ATOM	844	CD	ARG				29.708	27.492	6.616		45.29	A
	ATOM	845	NE	ARG				31.037	28.070	6.812		48.51	A
	MOTA	846	CZ	ARG				31.314	29.059	7.658		51.53	A
10	MOTA	847		ARG				30.355	29.593	8.406		53.75	A
10	ATOM	848		ARG				32.553	29.526	7.748		51.21	A
	MOTA	849	С	ARG				25.528	25.459	8.378		37.67	A
	MOTA	850	0	ARG				24.550	26.200	8.288		39.09	A
	MOTA	851	N			173		25.481	24.163	8.092		38.44	A
	ATOM	852	CA			173		24.259	23.528	7.619		39.25	A
15	ATOM	853	CB	LYS	Α	173	2	24.523	22.061	7.272	1.00	41.89	A
	ATOM	854	CG	LYS			2	23.279	21.298	6.830	1.00	45.52	A
	MOTA	855	CD	LYS	Α	173	2	23.557	19.808	6.653	1.00	49.60	A
	ATOM	856	CE	LYS	Α	173	- 2	24.477	19.530	5.469	1.00	52.63	A
	ATOM	857	NZ	LYS	Α	173	- 2	23.855	19.894	4.160	1.00	54.61	A
20	ATOM	858	C	LYS	Α	173	- 2	23.089	23.608	8.595	1.00	39.30	A
	ATOM	859	0	LYS	Α	173	- 2	21.981	23.960	8.201	1.00	39.62	A
	ATOM	860	N	ILE	А	174		23.320	23.282	9.863	1.00	37.96	A
	ATOM	861	CA			174		22.229	23.314	10.833		37.36	A
	ATOM	862	CB			174		22.159	21.998	11.652		37.44	A
25	ATOM	863		ILE				22.058	20.802	10.709		38.37	A
	ATOM	864		ILE				23.397	21.850	12.532		37.25	A
	ATOM	865		ILE				23.355	20.620	13.418		36.85	A
	ATOM	866	C			174		22.259	24.492	11.801		36.71	A
	ATOM	867	ŏ			174		21.448	24.556	12.724		38.05	A
30	ATOM	868	N			175		23.185	25.423	11.592		35.48	A
30	ATOM	869	CA			175		23.265	26.585	12.462		35.29	A
	ATOM	870	C			175		24.053	26.360	13.737		35.06	A
	ATOM	871	0			175		25.066	27.019	13.970		37.46	A
	MOTA	872	N			176		23.581	25.441	14.571		33.94	A
35	ATOM	873	CA			176		24.253	25.113	15.822		32.84	A
	ATOM	874	CB			176		23.938	26.155	16.901		33.54	A
	MOTA	875	OG			176		22.599	26.056	17.347		34.86	A
	MOTA	876	C			176		23.796	23.731	16.276		32.34	A
	MOTA	877	0			176		22.726	23.263	15.884		32.82	A
40	MOTA	878	N			177		24.609	23.085	17.103		29.39	A
	ATOM	879	CA			177		24.313	21.743	17.597		27.20	A
	MOTA	880	CB			177		25.621	20.989	17.865		26.39	A
	MOTA	881	CG	PHE	Α	177	2	26.372	20.585	16.622	1.00	26.18	A
	ATOM	882	CD1	PHE	Α	177	2	26.210	21.277	15.426	1.00	25.30	A
45	ATOM	883	CD2	PHE	Α	177	- 2	27.266	19.516	16.662	1.00	26.05	A
	ATOM	884	CE1	PHE	Α	177	2	26.923	20.912	14.290	1.00	26.59	A
	ATOM	885	CE2	PHE	Α	177	- 2	27.986	19.143	15.532	1.00	26.06	A
	ATOM	886	CZ	PHE	Α	177	- 2	27.815	19.841	14.343	1.00	25.42	A
	MOTA	887	C			177		23.500	21.752	18.884		27.00	A
50	ATOM	888	0			177		23.704	22.610	19.747		26.48	A
	ATOM	889	N	ASP				22.578	20.802	19.022		26.70	A
	ATOM	890	CA	ASP				21.816	20.729	20.260		26.35	A
	ATOM	891	CB	ASP				20.621	19.773	20.142		29.90	A
	ATOM	892	CG	ASP				21.020	18.372	19.720		32.28	A
55	ATOM	893		ASP				22.157	17.949	20.014		35.21	A
22	ATOM	894		ASP				20.179	17.683	19.105		34.79	A
	ATOM	895	C	ASP				22.810	20.228	21.311		25.03	A
	ATOM	896	0	ASP				23.974	19.968	20.992		21.24	A
		895	N			178			20.083			23.60	A A
	ATOM	89/	PI	다니	А	1/9	- 2	22.361	40.003	22.552	1.00	43.60	A

	ATOM	898	CA	GLU 2	Α	179	23.247	19.644	23.619	1.00	25.18	A
	ATOM	899	CB	GLU 2	А	179	22.542	19.770	24.971	1.00	27.60	A
	ATOM	900	CG	GLU 2			23.324	19.176	26.130		32.58	A
	ATOM	901	CD	GLU 2			22.997	19.845	27.449		35.82	A
5												
3	ATOM	902		GLU 2			21.825	20.224	27.645		35.95	A
	MOTA	903	OE2	GLU 2			23.912	19.984	28.291		38.19	A
	ATOM	904	C	GLU 2			23.808	18.235	23.450		24.08	A
	ATOM	905	0	GLU 2	A	179	24.977	17.989	23.756	1.00	22.79	A
	MOTA	906	N	THR 2	Α	180	22.983	17.316	22.961	1.00	23.36	A.
10	ATOM	907	CA	THR 2	Α	180	23.412	15.935	22.761	1.00	22.15	A
	ATOM	908	CB	THR 2	A	180	22,224	15.054	22.320	1.00	23.77	A
	ATOM	909	OG1	THR 2	A	180	21.222	15.075	23.341	1.00	26.37	A
	ATOM	910		THR			22.670	13.616	22.088		22.66	A
	ATOM	911	C	THR			24.533	15.830	21.724		22.01	A
15	ATOM	912	ŏ	THR I			25.533	15.141	21.944		19.87	A
13												
	MOTA	913	N	CYS			24.365	16.511	20.596		21.21	A.
	MOTA	914	CA	CYS			25.372	16.480	19.541		22.22	A
	MOTA	915	CB	CYS			24.800	17.065	18.250		24.62	A
	MOTA	916	SG	CYS	A	181	23.435	16.080	17.560	1.00	29.50	A
20	ATOM	917	C	CYS 2	Α	181	26.633	17.232	19.954	1.00	23.07	A
	ATOM	918	0	CYS 2	Α	181	27.746	16.827	19.608	1.00	23.95	A.
	ATOM	919	N	THR 2	Α	182	26.463	18.325	20.695	1.00	22.76	A
	ATOM	920	CA	THR 2	A	182	27.606	19.103	21.161	1.00	21.49	A
	ATOM	921	CB	THR			27.167	20.346	21.978		21.37	A
25	ATOM	922	OG1				26.459	21.262	21.134		22.50	A
23	ATOM	923	CG2	THR			28.379	21.046	22.565		18.36	Ā
	MOTA	924	С	THR I			28.454	18.215	22.071		21.48	A
	MOTA	925	0	THR I			29.669	18.090	21.894		19.95	A
	ATOM	926	N	ARG 2			27.798	17.602	23.050		18.97	A
30	MOTA	927	CA	ARG 2	A		28.468	16.723	23.996	1.00	19.39	A
	ATOM	928	CB	ARG		183	27.455	16.140	24.984	0.50	19.46	AC1
	ATOM	929	CG	ARG		183	28.030	15.062	25.887	0.50	18.77	AC1
	ATOM	930	CD	ARG		183	27.021	14.571	26.925	0.50	21.19	AC1
	ATOM	931	NE	ARG		183	26.605	15.642	27.824	0.50	19.46	AC1
35	ATOM	932	CZ	ARG		183	25.496	16.362	27.679		20.45	AC1
	ATOM	933		ARG		183	24.672	16.123	26.666		19.81	AC1
	ATOM	934		ARG		183	25.224	17.338	28.539		17.11	AC1
	ATOM	935	C	ARG I	70		29.206	15.577	23.302		20.02	A
		936	Ö									A
40	MOTA			ARG I			30.383	15.333	23.573		19.97	
40	MOTA	937	N	PHE 2			28.520	14.871	22.409		19.24	A
	MOTA	938	CA	PHE 2			29.144	13.746	21.722		18.04	A
	MOTA	939	CB	PHE 2			28.158	13.078	20.764		21.05	A
	MOTA	940	CG	PHE 2			28.719	11.857	20.098		22.67	A
	MOTA	941	CD1	PHE 2	A	184	28.717	10.630	20.754	1.00	22.97	A
45	MOTA	942	CD2	PHE 3	A	184	29.317	11.949	18.850	1.00	19.97	A
	ATOM	943	CE1	PHE 2	A	184	29.308	9.510	20.176	1.00	23.53	A
	ATOM	944	CE2	PHE 2	Α	184	29.915	10.833	18.263	1.00	24.11	A
	ATOM	945	CZ	PHE			29.910	9.613	18.928		22.97	A
	ATOM	946	c	PHE			30.403	14.127	20.941		17.99	A
50	ATOM	947	o	PHE			31.461	13.531	21.130		18.89	A
50	ATOM	948	N	TYR			30.292	15.110	20.056		15.73	A
	MOTA	949	CA	TYR 2			31.443	15.519	19.265		15.72	A
	MOTA	950	CB	TYR 2			30.992	16.413	18.111		17.33	A
	MOTA	951	CG	TYR 2			30.364	15.584	17.015		19.37	A
55	MOTA	952		TYR 2			31.159	14.809	16.168		16.53	A
	ATOM	953	CE1	TYR 2	Α	185	30.590	13.952	15.232	1.00	18.12	A
	ATOM	954	CD2	TYR 2	Α	185	28.976	15.484	16.892	1.00	18.18	A
	ATOM	955	CE2	TYR 2	Α	185	28.398	14.623	15.956	1.00	18.90	A
	ATOM	956	CZ	TYR			29.211	13.861	15.133		18.41	A
					-							

	ATOM	957	OH	TYR A	185	28.650	12.995	14.218	1.00 20.48	A
	ATOM	958	C	TYR A	185	32.544	16.172	20.083	1.00 15.79	A
	ATOM	959	0	TYR A	185	33.720	16.015	19.766	1.00 17.69	A
	ATOM	960	N	THR A	186	32.176	16.887	21.142	1.00 15.68	A
5	ATOM	961	CA	THR A		33.184	17.504	21.997	1.00 16.03	A
	MOTA	962	CB	THR A		32.559	18.403	23.094	1.00 16.62	A
	ATOM	963	OG1	THR A		31.866	19.503	22.481	1.00 14.79	A
	ATOM	964	CG2	THR A		33.656	18.953	24.019	1.00 14.68	A
	ATOM	965	C	THR A		33.954	16.375	22.680	1.00 15.59	A
10	ATOM	966	ō	THR A		35.176	16.443	22.823	1.00 13.77	A
10	ATOM	967	N	ALA A		33.234	15.333	23.097	1.00 14.06	A
	ATOM	968	CA	ALA A		33.869	14.196	23.757	1.00 14.74	A
	ATOM	969	CB	ALA A		32.810	13.195	24.224	1.00 14.74	A
	ATOM	970	C	ALA A		34.875	13.193	22.821	1.00 14.32	A
15	ATOM	971	0	ALA A		35.972	13.136	23.247	1.00 15.61	A
13	ATOM	972	N	GLU A		34.516	13.340	21.549	1.00 13.61	A
	ATOM	973	CA	GLU A		35.443	12.704	20.615	1.00 14.01	A
	ATOM	974	CB	GLU A		34.782	12.449	19.251	1.00 12.85	A
20	ATOM	975	CG	GLU A		33.622	11.454	19.282	1.00 12.71	A
20	ATOM	976	CD	GLU A		33.464	10.685	17.979	1.00 15.01	A
	MOTA	977		GLU A		33.687	11.275	16.899	1.00 13.21	A
	ATOM	978	OE2	GLU A		33.110	9.484	18.031	1.00 17.69	A
	ATOM	979	С	GLU A		36.682	13.582	20.436	1.00 13.34	A
	MOTA	980	0	GLU A		37.803	13.085	20.408	1.00 14.69	A
25	MOTA	981	N	ILE A		36.486	14.893	20.326	1.00 13.52	A
	MOTA	982	CA	ILE A		37.627	15.787	20.159	1.00 13.35	A
	ATOM	983	CB	ILE A		37.169	17.247	19.939	1.00 13.95	A
	ATOM	984		ILE A		38.381	18.165	19.822	1.00 12.47	A
	MOTA	985		ILE A		36.302	17.332	18.671	1.00 13.44	A
30	MOTA	986		ILE A		35.588	18.664	18.491	1.00 14.29	A
	MOTA	987	С	ILE A		38.530	15.702	21.394	1.00 14.63	A
	ATOM	988	0	ILE A		39.753	15.595	21.271	1.00 12.97	A
	MOTA	989	N	VAL A		37.927	15.751	22.582	1.00 14.35	A
	MOTA	990	CA	VAL A		38.684	15.655	23.832	1.00 13.22	A
35	MOTA	991	CB	VAL A		37.743	15.690	25.061	1.00 14.28	A
	MOTA	992		VAL A		38.509	15.267	26.326	1.00 15.08	A
	MOTA	993		VAL A		37.160	17.082	25.233	1.00 12.08	A
	MOTA	994	С	VAL A		39.468	14.338	23.859	1.00 14.61	A
	MOTA	995	0	VAL A		40.634	14.304	24.250	1.00 13.72	A
40	MOTA	996	N	SER A		38.825	13.254	23.432	1.00 15.26	A
	MOTA	997	CA	SER A		39.478	11.943	23.421	1.00 16.81	A
	MOTA	998	CB	SER	191	38.470	10.857	23.041	0.50 16.14	AC1
	ATOM	999	OG	SER	191	39.018	9.569	23.238	0.50 16.94	AC1
	MOTA	1000	C	SER A		40.649	11.928	22.441	1.00 16.58	A
45	MOTA	1001	0	SER A		41.697	11.335	22.713	1.00 13.96	A
	ATOM	1002	N	ALA A		40.468	12.586	21.300	1.00 15.26	A
	MOTA	1003	CA	ALA A		41.518	12.645	20.292	1.00 14.37	A
	MOTA	1004	CB	ALA A		40.989	13.296	19.016	1.00 14.43	A
	MOTA	1005	C	ALA A	192	42.695	13.440	20.845	1.00 16.46	A
50	MOTA	1006	0	ALA A	192	43.851	13.038	20.697	1.00 17.96	A
	MOTA	1007	N	LEU A	193	42.401	14.563	21.496	1.00 15.02	A
	MOTA	1008	CA	LEU A	193	43.459	15.392	22.067	1.00 15.42	A
	MOTA	1009	CB	LEU A	193	42.884	16.712	22.600	1.00 12.88	A
	ATOM	1010	CG	LEU A		42.445	17.721	21.525	1.00 15.97	A
55	MOTA	1011	CD1	LEU A	193	41.869	18.979	22.190	1.00 13.97	A
	MOTA	1012		LEU A		43.642	18.088	20.655	1.00 14.58	A
	MOTA	1013	C	LEU A		44.211	14.659	23.174	1.00 14.49	A
	ATOM	1014	0	LEU A		45.427	14.813	23.310	1.00 16.56	A
	ATOM	1015	N	GLU A	194	43.500	13.870	23.975	1.00 13.96	A

	3.0001	1016		GLU		104	44.179	13.123	25.032	1 00	14.08	
	ATOM	1016	CA									A
	MOTA	1017	CB	GLU	Α	194	43.190	12.295	25.857	1.00	14.65	A
	MOTA	1018	CG	GLU	Α	194	43.882	11.301	26.789	1.00	17.09	A
	ATOM	1019	CD	GLU			42.924	10.592	27.730	1 00	19.59	A
5												
3	ATOM	1020		GLU			41.809	10.237	27.295		19.25	A
	MOTA	1021	OE2	GLU			43.302	10.380	28.906	1.00	20.20	A
	ATOM	1022	C	GLU	Α	194	45.208	12.199	24.386	1.00	13.57	A
	ATOM	1023	0	GLU	Δ	194	46.337	12.093	24.847	1 00	14.23	A
	ATOM	1024	N	TYR			44.822	11.544	23.301		14.89	A
10	MOTA	1025	CA	TYR			45.743	10.642	22.618		16.58	A
	MOTA	1026	CB	TYR	Α	195	45.030	9.910	21.488	1.00	17.29	A
	ATOM	1027	CG	TYR	Α	195	45.956	9.058	20.649	1.00	17.92	A
	ATOM	1028		TYR			46.347	7.788	21.077		17.96	A
	ATOM	1029		TYR			47.203	6.996	20.304		19.77	A
15	MOTA	1030		TYR			46.445	9.524	19.428		16.67	A
	MOTA	1031	CE2	TYR	Α	195	47.299	8.744	18.650	1.00	18.51	A
	ATOM	1032	CZ	TYR	Α	195	47.671	7.481	19.094	1.00	20.24	A
	ATOM	1033	OH	TYR	А	195	48.506	6.705	18.325	1.00	21.89	A
	ATOM	1034	C	TYR			46.917	11.419	22.035		16.98	A
20												
20	MOTA	1035	0	TYR			48.081	11.047	22.203		14.61	A
	MOTA	1036	N	LEU	Α	196	46.599	12.507	21.347	1.00	16.30	A
	ATOM	1037	CA	LEU	Α	196	47.619	13.328	20.720	1.00	18.15	A
	ATOM	1038	CB	LEU	А	196	46.969	14.502	19.982	1.00	18.59	A
	ATOM	1039	CG	LEU			47.834	15.203	18.935		22.51	A
25				LEU								
23	MOTA	1040					48.222	14.206	17.841		20.94	A
	ATOM	1041	CD2	LEU			47.060	16.375	18.338		22.98	A
	MOTA	1042	C	LEU	Α	196	48.592	13.844	21.763	1.00	17.75	A
	ATOM	1043	0	LEU	Α	196	49.801	13.644	21.649	1.00	18.33	A
	MOTA	1044	N	HIS			48.064	14.495	22.792		17.12	A
30	ATOM	1045	CA	HIS			48.913	15.042	23.842		18.47	A
30												
	ATOM	1046	CB	HIS			48.069	15.866	24.817		15.90	A
	MOTA	1047	CG	HIS	Α	197	47.571	17.152	24.231	1.00	19.15	A
	ATOM	1048	CD2	HIS	Α	197	47.830	17.745	23.038	1.00	18.22	A
	ATOM	1049	ND1	HIS	А	197	46.704	17.992	24.897	1.00	17.47	A
35	ATOM	1050		HIS			46.450	19.047	24.139		19.74	A
55												
	MOTA	1051		HIS			47.119	18.921	23.007		15.69	A
	MOTA	1052	С	HIS			49.696	13.958	24.572		19.40	A
	MOTA	1053	0	HIS	Α	197	50.823	14.192	25.021	1.00	19.42	A
	ATOM	1054	N	GLY	Α	198	49.106	12.770	24.679	1.00	18.59	A
40	ATOM	1055	CA	GLY			49.793	11.675	25.339		19.60	A
	ATOM	1056	C	GLY			51.075	11.307	24.612		21.86	A
	MOTA	1057	0	GLY			51.963	10.682	25.186		23.09	A
	MOTA	1058	N	LYS	Α	199	51.174	11.687	23.341	1.00	22.81	A
	ATOM	1059	CA	LYS	Α	199	52.368	11.401	22.549	1.00	24.43	A
45	ATOM	1060	CB	LYS	А	199	51.990	10.905	21.154	1.00	26.00	A
	ATOM	1061	CG	LYS			51.378	9.520	21.133		30.98	A
	MOTA	1062	CD	LYS			51.291	9.002	19.708		36.85	A
	MOTA	1063	CE	LYS	Α	199	50.832	7.559	19.682	1.00	40.37	A
	ATOM	1064	NZ	LYS	Α	199	51.646	6.691	20.581	1.00	43.48	A
50	ATOM	1065	С	LYS	Α	199	53.253	12.631	22.414	1.00	23.88	A
	ATOM	1066	ō	LYS			54.144	12.669	21.568		24.97	A
	MOTA	1067	N	GLY			52.997	13.638	23.243		24.00	A
	MOTA	1068	CA	GLY			53.790	14.853	23.203	1.00	22.12	A
	ATOM	1069	C	GLY	Α	200	53.665	15.632	21.907	1.00	22.14	A
55	ATOM	1070	0	GLY			54.632	16.231	21.439		22.41	A
	ATOM	1071	N	ILE			52.475	15.630	21.320		20.00	A
	ATOM	1072	CA	ILE			52.252	16.355	20.080		18.93	A
	MOTA	1073	CB	ILE			51.784	15.414	18.955		19.70	A
	MOTA	1074	CG2	ILE	Α	201	51.414	16.226	17.716	1.00	20.12	A

	MOTA	1075	CG1	ILE	Α	201	52.880	14.395	18.636	1.00	20.03	A
	ATOM	1076	CD1	ILE	Α	201	52.408	13.258	17.745	1.00	22.75	A
	ATOM	1077	C			201	51.193	17.425	20.270		19.87	A
_	MOTA	1078	0	ILE			50.121	17.161	20.817		20.08	A
5	ATOM	1079	N	ILE			51.508	18.633	19.815		19.94	A
	MOTA	1080	CA	ILE	Α	202	50.601	19.772	19.891	1.00	20.45	A
	ATOM	1081	CB	ILE	Α	202	51.352	21.040	20.356	1.00	22.21	A
	ATOM	1082	CG2	ILE	А	202	50.381	22.220	20.470		22.67	A
	ATOM	1083		ILE			52.033	20.775	21.700		24.19	A
10	ATOM	1084		ILE			52.914	21.920	22.169		25.39	A
10												
	MOTA	1085	C	ILE			50.105	19.999	18.464		20.71	A
	ATOM	1086	0	ILE	Α	202	50.910	20.067	17.538	1.00	19.48	A
	MOTA	1087	N	HIS	Α	203	48.795	20.108	18.270	1.00	18.65	A
	ATOM	1088	CA	HIS	Α	203	48.280	20.319	16.919	1.00	18.02	A
15	ATOM	1089	CB	HIS	А	203	46.775	20.057	16.874	1.00	16.31	A
	ATOM	1090	CG	HIS			46.199	20.136	15.495		18.36	A
	ATOM	1091		HIS			46.043	21.186	14.655		16.42	A
	MOTA	1092		HIS			45.759	19.026	14.806		19.50	A
	MOTA	1093	CE1	HIS	Α	203	45.359	19.389	13.600	1.00	17.64	A
20	MOTA	1094	NE2	HIS	Α	203	45.522	20.694	13.483	1.00	20.87	A
	ATOM	1095	C	HIS	Α	203	48.589	21.738	16.405	1.00	18.92	A
	ATOM	1096	0	HIS	А	203	49.073	21.906	15.282	1.00	16.21	A
	ATOM	1097	N	ARG			48.301	22.744	17.232		18.60	A
	ATOM	1098	CA	ARG			48.552	24.157	16.914		19.81	A
25			CB	ARG			49.998	24.365	16.458		21.61	A
23	ATOM	1099										
	MOTA	1100	CG	ARG			51.024	24.137	17.550		23.82	A
	MOTA	1101	CD	ARG			52.323	24.870	17.252		27.62	A
	MOTA	1102	NE	ARG	Α	204	52.932	24.449	15.994	1.00	29.43	A
	MOTA	1103	CZ	ARG	Α	204	54.125	24.861	15.572	1.00	33.10	A
30	ATOM	1104	NH1	ARG	Α	204	54.835	25.706	16.311	1.00	32.12	A
	ATOM	1105	NH2	ARG	А	204	54.614	24.426	14.418	1.00	30.25	A
	ATOM	1106	C	ARG			47.624	24.830	15.905		20.03	A
	ATOM	1107	ō	ARG			47.711	26.038	15.698		20.88	A
	ATOM	1107	N	ASP			46.755	24.071	15.255		18.96	A
2.5												
35	MOTA	1109	CA	ASP			45.828	24.692	14.325		17.90	A
	MOTA	1110	CB	ASP			46.418	24.741	12.914		18.95	A
	MOTA	1111	CG	ASP	Α	205	45.655	25.688	12.008	1.00	20.36	A
	MOTA	1112	OD1	ASP	Α	205	44.939	26.560	12.545	1.00	20.35	A
	ATOM	1113	OD2	ASP	Α	205	45.772	25.573	10.771	1.00	22.49	A
40	ATOM	1114	C	ASP	Α	205	44.500	23.956	14.328	1.00	19.60	A
	ATOM	1115	0	ASP	Δ	205	43.876	23.751	13.287	1 00	21.53	A
	ATOM	1116	N	LEU			44.063	23.569	15.521		18.53	A
	ATOM	1117	CA	LEU			42.813	22.851	15.667		19.18	A
	MOTA	1118	CB	LEU			42.693	22.295	17.087		18.94	A
45	MOTA	1119	CG	LEU			41.511	21.358	17.346		23.10	A
	ATOM	1120	CD1	LEU	Α	206	41.615	20.142	16.436	1.00	23.01	A
	MOTA	1121	CD2	LEU	Α	206	41.504	20.933	18.808	1.00	22.97	A
	ATOM	1122	C	LEU	Α	206	41.639	23.772	15.361	1.00	19.05	A
	ATOM	1123	0	LEU	Α	206	41.556	24.880	15.886	1.00	19.25	A
50	ATOM	1124	N	LYS			40.740	23.307	14.500		17.54	A
	ATOM	1125	CA	LYS			39.564	24.081	14.110		18.60	A
	ATOM	1126	CB	LYS			39.980	25.248	13.196		18.98	A
	MOTA	1127	CG	LYS			40.786	24.817	11.982		18.20	A
	MOTA	1128	CD	LYS			41.246	26.000	11.139		21.42	A
55	MOTA	1129	CE	LYS			42.223	25.537	10.062		23.21	A
	MOTA	1130	NZ	LYS	Α	207	42.561	26.604	9.084	1.00	29.61	A
	ATOM	1131	C	LYS	Α	207	38.566	23.181	13.388	1.00	18.18	A
	ATOM	1132	0	LYS	Α	207	38.921	22.100	12.915	1.00	18.11	A
	ATOM	1133	N	PRO			37.298	23.614	13.293		20.26	A

	ATOM	1134	CD	PRO	Α	208	36.713	24.833	13.882	1.00	18.79	A
	ATOM	1135	CA	PRO	А	208	36.272	22.814	12.616	1.00	19.67	A
	MOTA	1136	CB	PRO	Α	208	35.063	23.742	12.608	1.00	19.45	A
	ATOM	1137	CG			208	35.231	24.509	13.891		21.81	A
5	ATOM	1138	C			208	36.674	22.372	11.209		21.04	A
	ATOM	1139	ŏ			208	36.264	21.307	10.751		21.19	A
	ATOM	1140	N			209	37.474	23.188	10.731		21.69	A
	ATOM	1141	CA		А	209	37.928	22.872	9.170		22.64	A
10	ATOM	1142	CB	GLU		209	38.644	24.084	8.558		23.65	AC1
10	MOTA	1143	CG	GLU		209	39.253	23.825	7.185		27.24	AC1
	MOTA	1144	CD	GLU		209	40.155	24.958	6.716		29.40	AC1
	ATOM	1145		GLU		209	39.660	26.094	6.553		29.68	AC1
	MOTA	1146	OE2	GLU		209	41.363	24.711	6.511	0.50	30.07	AC1
	ATOM	1147	C	GLU	Α	209	38.879	21.668	9.159	1.00	22.28	A
15	ATOM	1148	0	GLU	Α	209	38.955	20.933	8.170	1.00	21.36	A.
	ATOM	1149	N	ASN	Α	210	39.600	21.490	10.263	1.00	19.90	A
	MOTA	1150	CA	ASN	Α	210	40.574	20.412	10.436	1.00	19.44	A
	ATOM	1151	CB	ASN			41.744	20.912	11.287	1.00	20.07	A
	ATOM	1152	CG	ASN			42.746	21.698	10.479		25.77	A.
20	ATOM	1153		ASN			43.571	22.427	11.029		26.73	A
20	ATOM	1154		ASN			42.687	21.548	9.158		25.15	A
	ATOM	1155	C	ASN			40.005	19.151	11.078		18.63	A
	ATOM	1156	0	ASN			40.712	18.154	11.234		18.29	A
		1157				211	38.739	19.202	11.469		16.31	A
2.5	MOTA		N									
25	ATOM	1158	CA			211	38.090	18.058	12.085		15.49	A
	MOTA	1159	CB			211	37.336	18.488	13.354		15.40	A
	MOTA	1160		ILE			36.582	17.311	13.950		14.59	A
	MOTA	1161		ILE			38.342	19.046	14.365		15.91	A.
	MOTA	1162		ILE			37.720	19.669	15.590		15.98	A.
30	MOTA	1163	C			211	37.131	17.485	11.059		17.26	A.
	MOTA	1164	0			211	35.995	17.947	10.926		18.16	A.
	ATOM	1165	N	LEU	Α	212	37.599	16.486	10.317	1.00	15.97	A
	MOTA	1166	CA	LEU	Α	212	36.784	15.875	9.274	1.00	17.08	A
	MOTA	1167	CB	LEU	Α	212	37.685	15.249	8.202	1.00	17.78	A
35	ATOM	1168	CG	LEU	Α	212	38.785	16.157	7.640	1.00	18.92	A.
	ATOM	1169	CD1	LEU	А	212	39.476	15.450	6.485	1.00	22.09	A.
	ATOM	1170	CD2	LEU	А	212	38.188	17.482	7.166	1.00	19.91	A
	ATOM	1171	С			212	35.843	14.825	9.837		18.35	A
	ATOM	1172	o			212	35.957	14.433	11.002		19.39	A
40	ATOM	1173	N			213	34.915	14.368	9.000		17.84	A
40	ATOM	1174	CA			213	33.942	13.362	9.403		19.94	A
	ATOM	1175	CB			213	32.556	14.004	9.487		20.84	A
	ATOM	1176	CG			213	32.396	15.059	10.583		20.31	A
	ATOM	1177		LEU			31.124	15.837	10.367		22.75	A.
45	MOTA	1178		LEU			32.379	14.378	11.940		23.93	A
	MOTA	1179	C			213	33.914	12.187	8.426		20.98	A
	MOTA	1180	0			213	33.743	12.379	7.218		19.55	A.
	MOTA	1181	N	ASN			34.088	10.970	8.935		20.44	A.
	MOTA	1182	CA	ASN	Α	214	34.055	9.814	8.049	1.00	23.77	A
50	MOTA	1183	CB	ASN	Α	214	34.745	8.596	8.674	1.00	25.30	A
	ATOM	1184	CG	ASN	Α	214	34.077	8.127	9.948	1.00	32.04	A
	MOTA	1185	OD1	ASN	Α	214	32.908	8.422	10.206	1.00	34.43	A.
	ATOM	1186		ASN			34.818	7.369	10.752	1.00	33.85	A
	ATOM	1187	C	ASN			32.618	9.466	7.693		24.07	A
55	ATOM	1188	0	ASN			31.672	10.113	8.150		19.94	A
	ATOM	1189	N			215	32.459	8.433	6.879		25.77	A
	ATOM	1190	CA			215	31.138	8.003	6.445		28.69	A
	ATOM	1190	CB			215	31.275	6.796	5.513		31.98	A
		1191	CG									A
	ATOM	1192	UG:	CTIO	А	215	29.970	6.334	4.896	1.00	40.22	A

	ATOM	1193	CD	GLU	А	215	30.182	5.312	3.795	1.00	44.27	A
	ATOM	1194	OF1	GLU			30.817	4.268	4.065	1 00	46.46	A
	MOTA	1195		GLU			29.716	5.556	2.660		46.13	A
	MOTA	1196	C			215	30.188	7.673	7.601		28.41	A
5	ATOM	1197	0	GLU	Α	215	28.971	7.769	7.447	1.00	28.52	A
	MOTA	1198	N	ASP	Α	216	30.737	7.287	8.752	1.00	26.77	A
	ATOM	1199	CA	ASP	Δ	216	29.914	6.953	9.917	1.00	27.28	A
	ATOM	1200	CB	ASP			30.538	5.795	10.696		31.27	A
	ATOM	1201	CG	ASP			30.390	4.466	9.979		37.61	A
10												
10	MOTA	1202		ASP			29.274	4.170	9.499		39.45	A
	MOTA	1203		ASP			31.382	3.710	9.902		41.84	A
	MOTA	1204	С	ASP	Α	216	29.697	8.135	10.862	1.00	26.37	A
	MOTA	1205	0	ASP	Α	216	29.136	7.984	11.950	1.00	25.73	A
	ATOM	1206	N	MET	А	217	30.156	9.306	10.441	1.00	23.02	A
15	ATOM	1207	CA	MET			30.015	10.527	11.218		21.83	A
15	ATOM	1208	CB	MET			28.537	10.789	11.517		23.24	A
	MOTA	1209	CG	MET			27.742	11.186	10.274		22.98	A
	MOTA	1210	SD	MET			28.464	12.616	9.430		27.57	A
	ATOM	1211	CE	MET	Α	217	27.679	13.974	10.332	1.00	26.68	A
20	MOTA	1212	C	MET	Α	217	30.844	10.618	12.502	1.00	21.51	A
	ATOM	1213	0	MET	Α	217	30.474	11.323	13.440	1.00	18.62	A
	ATOM	1214	N	HIS	А	218	31.957	9.892	12.544	1.00	20.10	A
	ATOM	1215	CA	HIS			32.873	9.964	13.678		19.86	A
	ATOM	1216	CB	HIS			33.482	8.594	13.977		20.21	A
25				HIS				7.667				
23	ATOM	1217	CG				32.551		14.698		22.40	A
	MOTA	1218		HIS			31.910	6.547	14.287		21.27	A
	MOTA	1219		HIS			32.177	7.863	16.011		19.59	A
	MOTA	1220	CE1	HIS	Α	218	31.348	6.902	16.379	1.00	21.88	A
	ATOM	1221	NE2	HIS	Α	218	31.168	6.091	15.351	1.00	22.08	A
30	ATOM	1222	C	HIS	Α	218	33.947	10.921	13.172	1.00	19.10	A
	ATOM	1223	0	HIS	А	218	34.170	11.004	11.965	1.00	20.31	A
	ATOM	1224	N	ILE			34.617	11.638	14.067		17.21	A
	ATOM	1225	CA	ILE			35.628	12.586	13.618		15.26	A
	ATOM	1226	CB	ILE			35.987	13.614	14.716		15.38	A
2.5												
35	MOTA	1227		ILE			34.722	14.305	15.221		14.58	A
	MOTA	1228		ILE			36.734	12.919	15.864		14.46	A
	MOTA	1229	CD1	ILE	Α	219	37.279	13.885	16.911	1.00	13.74	A
	MOTA	1230	С	ILE	Α	219	36.929	11.944	13.161	1.00	16.21	A
	ATOM	1231	0	ILE	Α	219	37.238	10.799	13.500	1.00	15.88	A
40	ATOM	1232	N	GLN	Α	220	37.677	12.711	12.378	1.00	15.62	A
	ATOM	1233	CA	GLN	A	220	38.980	12.316	11.876	1.00	17.84	A
	ATOM	1234	СВ	GLN			38.872	11.595	10.525		20.00	A
	ATOM	1235	CG	GLN			38.463	10.129	10.659		26.97	A
	ATOM	1236	CD	GLN			38.648	9.343	9.372		29.95	A
4.5												
45	ATOM	1237		GLN			37.968	9.590	8.373		33.12	A
	MOTA	1238		GLN			39.578	8.393	9.389		30.47	A
	MOTA	1239	С	GLN	Α	220	39.757	13.610	11.735	1.00	17.00	A
	MOTA	1240	0	GLN	Α	220	39.609	14.339	10.751	1.00	18.27	A
	MOTA	1241	N	ILE	Α	221	40.566	13.906	12.746	1.00	14.34	A
50	MOTA	1242	CA	ILE	Α	221	41.361	15.120	12.753	1.00	14.46	A
	ATOM	1243	СВ	ILE			41.867	15.416	14.175		12.30	A
	ATOM	1244		ILE			42.764	16.656	14.167		14.78	A
	ATOM	1245		ILE			40.660	15.613	15.102		13.92	A
	ATOM	1246		ILE			41.003	15.901	16.543		15.06	A
55	MOTA	1247	С			221	42.536	14.996	11.783		15.44	A
	MOTA	1248	0	ILE			43.106	13.915	11.613		13.93	A
	MOTA	1249	N	THR			42.877	16.101	11.127		15.36	A
	MOTA	1250	CA	THR	Α	222	43.980	16.098	10.174	1.00	17.52	A
	MOTA	1251	CB	THR	Α	222	43.470	15.836	8.750	1.00	19.92	A

	ATOM	1252	OG1	THR	Α	222	44.587	15.637	7.875	1.00	18.78	A
	ATOM	1253	cco	THR	70	222	42.630	17.018	8.257	1 00	18.16	A
	ATOM	1254	C	THR			44.735	17.428	10.192		19.60	A
	ATOM	1255	0	THR	Α	222	44.509	18.257	11.084	1.00	18.59	A
5	ATOM	1256	N	ASD	Z.	223	45.630	17.610	9.216	1 00	18.69	A
-												
	MOTA	1257	CA	ASP			46.440	18.825	9.069		20.12	A
	ATOM	1258	CB	ASP	Α	223	45.532	20.065	9.108	1.00	23.51	A
	ATOM	1259	CG	ASP	Δ	223	46.248	21.335	8.670	1 00	27.09	A
	ATOM	1260		ASP			47.283	21.227	7.975		26.28	A
10	MOTA	1261	OD2	ASP	Α	223	45.765	22.438	9.009	1.00	26.15	A
	ATOM	1262	C	ASP	А	223	47.516	18.913	10.150	1.00	21.73	A
	ATOM	1263	ō	ASP			47.439	19.751	11.055		22.76	A
	MOTA	1264	N	PHE			48.535	18.063	10.027		20.75	A
	ATOM	1265	CA	PHE	Α	224	49.611	17.988	11.009	1.00	20.11	A
15	ATOM	1266	CB	PHE	A	224	49.805	16.527	11.424	1.00	20.62	A
	ATOM	1267	CG	PHE			48.682	15.991	12.263		21.41	A
	MOTA	1268	CD1	PHE	Α	224	48.598	16.312	13.614	1.00	23.05	A
	ATOM	1269	CD2	PHE	А	224	47.681	15.212	11.693	1.00	22.27	A
	ATOM	1270		PHE			47.528	15.868	14.389		23.30	A
20												
20	ATOM	1271	CE2	PHE			46.606	14.763	12.457		21.11	A
	ATOM	1272	CZ	PHE	Α	224	46.530	15.093	13.807	1.00	22.02	A
	MOTA	1273	C	PHE	A	224	50.957	18.583	10.619	1.00	20.45	A
	MOTA	1274	0	PHE			51.905	18.547	11.407		20.73	A
	ATOM	1275	N	GLY	А	225	51.049	19.125	9.412	1.00	22.02	A
25	ATOM	1276	CA	GLY	А	225	52.301	19.713	8.981	1.00	22.66	A
	ATOM	1277	C			225	52.742	20.822	9.920		24.99	A
	MOTA	1278	0	GLY			53.939	21.041	10.122	1.00	24.52	A
	ATOM	1279	N	THR	Α	226	51.779	21.524	10.508	1.00	23.50	A
	ATOM	1280	CA	THR	А	226	52.106	22.613	11.416	1.00	25.16	A
30	ATOM	1281	CB	THR				23.829	11.160		24.76	A
30							51.199					
	ATOM	1282	OG1	THR	A	226	49.831	23.410	11.113	1.00	22.68	A
	ATOM	1283	CG2	THR	А	226	51.571	24.490	9.834	1.00	25.00	A
	ATOM	1284	C			226	52.046	22.233	12.894		25.79	A
	MOTA	1285	0			226	52.019	23.100	13.768		24.54	A
35	ATOM	1286	N	ALA	Α	227	52.037	20.935	13.173	1.00	24.97	A
	ATOM	1287	CA	ALA	Α	227	52.004	20.475	14.550	1.00	25.49	A
	ATOM	1288	СВ	ALA			51.659	18.993	14.607		22.85	A
	MOTA	1289	C	ALA			53.384	20.715	15.149		27.70	A
	ATOM	1290	0	ALA	A	227	54.331	21.047	14.435	1.00	26.60	A
40	ATOM	1291	N	LYS	Δ	228	53.491	20.558	16.461	1 00	28.53	A
	ATOM	1292	CA	LYS			54.760	20.745	17.149		32.12	A
	MOTA	1293	CB	LYS	Α	228	54.699	21.974	18.054	1.00	33.81	A
	ATOM	1294	CG	LYS	А	228	56.007	22.294	18.765	1.00	41.23	A
	ATOM	1295	CD	LYS	75	228	57.082	22.725	17.768	1 00	47.57	A
4.5												
45	MOTA	1296	CE	LYS			58.401	23.056	18.462		49.82	A
	MOTA	1297	NZ	LYS	A	228	59.459	23.425	17.480	1.00	51.49	A
	ATOM	1298	С	LYS	Δ	228	55.019	19.504	17.985	1.00	33.25	A
	ATOM	1299	ō	LYS			54.190	19.129	18.815		33.70	A
	MOTA	1300	N	VAL	Α	229	56.159	18.860	17.756	1.00	33.64	A
50	ATOM	1301	CA	VAL	Α	229	56.516	17.661	18.501	1.00	34.66	A
	ATOM	1302	СВ	VAL			57.248	16.646	17.609		33.50	A
	MOTA	1303		VAL			57.619	15.419	18.415		32.34	A
	ATOM	1304	CG2	VAL	Α	229	56.370	16.264	16.436	1.00	34.25	A
	ATOM	1305	C	VAL	Α	229	57.420	18.035	19.668	1.00	37.57	A
55		1306	o	VAL					19.474		35.91	A
33	ATOM						58.581	18.392				
	ATOM	1307	N	LEU			56.877	17.948	20.878		40.57	A
	ATOM	1308	CA	LEU	Α	230	57.615	18.289	22.088	1.00	46.10	A
	ATOM	1309	CB	LEU			56.654	18.417	23.270		44.71	A
												A
	MOTA	1310	CG	LEU	А	430	55.627	19.545	23.207	1.00	44.50	A

	ATOM	1311	CD1	LEU	А	230	54.673	19.430	24.383	1.00	44.39	A
	ATOM	1312	CD2	LEU	Α	230	56.340	20.885	23.214	1.00	44.81	A
	ATOM	1313	C			230	58.695	17.279	22,440		50.42	A
	ATOM	1314	0	LEU	А	230	58.603	16.104	22.089	1.00	51.64	A
5	ATOM	1315	N	SER	А	231	59.717	17.756	23.145	1.00	55.81	A
	ATOM	1316	CA	SER			60.824	16.914	23.583		61.14	A
	ATOM	1317	CB	SER			62.077	17.200	22.750		61.27	A
	ATOM	1318	OG	SER	Α	231	62.444	18.568	22.823	1.00	62.85	A
	ATOM	1319	С	SER	Δ	231	61.124	17.126	25.071	1 00	64.65	A
10												
10	MOTA	1320	0			231	61.392	16.164	25.794		65.70	A
	MOTA	1321	N	PRO	Α	232	61.081	18.387	25.549	1.00	67.54	A
	ATOM	1322	CD	PRO	А	232	60.854	19.651	24.823	1.00	68.60	A
	ATOM	1323	CA	PRO			61.358	18.655	26.966		68.74	A
	MOTA	1324	CB	PRO			61.109	20.158	27.086		68.83	A
15	ATOM	1325	CG	PRO	Α	232	61.505	20.666	25.737	1.00	68.96	A
	ATOM	1326	С	PRO	A	232	60.460	17.846	27.899	1.00	69.17	A
	ATOM	1327	ō	PRO			59.335	17.494	27.541		69.94	A
	MOTA	1328	N	ALA	Α	237	57.424	23.198	27.637	1.00	80.06	A
	ATOM	1329	CA	ALA	Α	237	56.783	23.047	26.335	1.00	79.29	A
20	ATOM	1330	CB	ALA			55.275	22.907	26.512		78.64	A
20												
	MOTA	1331	C	ALA			57.092	24.239	25.433		79.07	A
	ATOM	1332	0	ALA	Α	237	56.250	25.113	25.249	1.00	79.47	A
	ATOM	1333	N	ALA	A	238	58.297	24.280	24.871	1.00	78.57	A
	ATOM	1334	CA	ALA			58.683	25.383	23.992		78.50	A
25	ATOM	1335	CB	ALA	А	238	60.186	25.347	23.728	1.00	78.50	A
	ATOM	1336	C	ALA	Α	238	57.920	25.327	22.673	1.00	78.15	A
	ATOM	1337	0	ALA	Δ	238	57.243	24.341	22.375	1.00	77.96	A
	MOTA	1338	N	ALA			58.027	26.393	21.887		77.28	A
	ATOM	1339	CA	ALA	А	239	57.338	26.452	20.603	1.00	76.27	A
30	ATOM	1340	CB	ALA	А	239	55.849	26.489	20.827	1.00	76.61	A
	ATOM	1341	C	ALA			57.766	27.667	19.793		75.38	A
	ATOM	1342	0	ALA			58.955	27.955	19.700		75.89	A
	ATOM	1343	N	ASN	Α	240	56.781	28.357	19.214	1.00	73.95	A
	MOTA	1344	CA	ASN	Δ	240	56.967	29.553	18.389	1 00	71.07	A
35		1345									71.47	
33	ATOM		CB	ASN			58.151	30.400	18.874			A
	MOTA	1346	CG	ASN			59.459	30.055	18.174		72.06	A
	ATOM	1347	OD1	ASN	А	240	59.575	30.149	16.943	1.00	72.03	A
	ATOM	1348	MD2	ASN	70	240	60.470	29.665	18.964	1 00	71.91	A
	MOTA	1349	C	ASN			57.188	29.178	16.928		69.41	A
40	ATOM	1350	0	ASN	Α	240	57.480	28.024	16.624	1.00	70.09	A
	ATOM	1351	N	ALA	Α	241	57.055	30.165	16.038	1.00	66.62	A
	ATOM	1352	CA	ALA			57.246	30.013	14.585		63.94	A
	ATOM	1353	C	ALA			55.952	30.080	13.772		60.63	A
	ATOM	1354	0	ALA	A	241	55.840	30.880	12.845	1.00	61.29	A
45	ATOM	1355	CB	ALA	А	241	57.979	28.704	14.246	1.00	65.23	A
	MOTA	1356	N	PHE			54.984	29.236	14.113		56.72	A
	MOTA	1357	CA	PHE	Α	242	53.712	29.196	13.394	1.00	52.53	A
	ATOM	1358	CB	PHE	A	242	53.419	27.767	12.923	1.00	49.14	A
	ATOM	1359	CG	PHE			52.040	27.590	12.354		47.38	A
50												
50	MOTA	1360		PHE			51.731	28.067	11.085		47.69	A
	MOTA	1361	CD2	PHE	Α	242	51.038	26.975	13.102	1.00	45.45	A
	MOTA	1362	CE1	PHE	А	242	50.445	27.937	10.565	1.00	46.75	A
	MOTA	1363		PHE			49.751	26.840	12.594		45.41	A
	ATOM	1364	CZ	PHE	Α	242	49.453	27.323	11.322	1.00	46.55	A
55	ATOM	1365	С	PHE	Α	242	52.534	29.688	14.229	1.00	50.08	A
	MOTA	1366	ō	PHE			52.502	29.505	15.444		49.86	A
	MOTA	1367	N			243	51.566	30.305	13.557		47.67	A
	ATOM	1368	CA	VAL	Α	243	50.355	30.809	14.200	1.00	46.21	A
	ATOM	1369	CB	VAL	Α	243	50.340	32.352	14.258	1.00	47.36	A
					-							

	ATOM	1370	CG1	VAL A	243	49.012	32.844	14.825	1.00	47.54	Α
	ATOM	1371		VAL A		51.497	32.842	15.109		48.50	A
	ATOM	1372	C	VAL A		49.150	30.342	13.389		44.12	A
	ATOM	1373	ō	VAL A		48.956	30.765	12.247		44.46	A
5		1374		GLY A							
3	ATOM		N			48.348	29.467	13.985		40.48	A
	MOTA	1375	CA	GLY A		47.176	28.941	13.306		37.65	A
	ATOM	1376	C	GLY A		46.101	29.960	12.964		35.39	A
	MOTA	1377	0	GLY A		46.313	31.168	13.065		35.92	A
	MOTA	1378	N	THR A	245	44.936	29.463	12.560	1.00	33.30	A
10	ATOM	1379	CA	THR A	245	43.813	30.312	12.184	1.00	30.20	A
	MOTA	1380	CB	THR A	245	42.593	29.450	11.829	1.00	32.00	A
	ATOM	1381	OG1	THR A	245	42.952	28.573	10.755	1.00	32.81	A
	ATOM	1382		THR A		41.419	30.319	11.390		28.34	A
	ATOM	1383	С	THR A		43.476	31.296	13.296		27.96	A
15	ATOM	1384	ō	THR A		43.212	30.907	14.434		25.46	A
	ATOM	1385	N	ALA A		43.486	32.576	12.938		25.22	A
	ATOM	1386	CA	ALA A		43.247	33.675	13.867		23.27	A
		1387	CB								
	MOTA			ALA A		42.956	34.955	13.082		22.94	A
	MOTA	1388	C	ALA A		42.178	33.475	14.934		21.27	A
20	MOTA	1389	0	ALA A		42.431	33.705	16.114		20.93	A
	MOTA	1390	N	GLN A		40.988	33.047	14.536		19.67	A
	MOTA	1391	CA	GLN A		39.911	32.886	15.504		20.17	A
	ATOM	1392	CB	GLN	247	38.608	32.535	14.779	0.50	21.89	AC1
	MOTA	1393	CG	GLN	247	38.522	33.076	13.355	0.50	26.18	AC1
25	ATOM	1394	CD	GLN	247	37.220	33.794	13.064	0.50	27.30	AC1
	ATOM	1395	OE1	GLN	247	36.172	33.447	13.605	0.50	30.13	AC1
	ATOM	1396	NE2	GLN	247	37.278	34.792	12.189	0.50	28.70	AC1
	ATOM	1397	С	GLN A		40.181	31.849	16.595		19.43	A
	ATOM	1398	ō	GLN A		39.546	31.883	17.648		18.93	A
30	ATOM	1399	N	TYR A		41.132	30.948	16.359		18.60	A
50	ATOM	1400	CA	TYR A		41.441	29.896	17.329		19.20	A
			CB								
	ATOM	1401		TYR A		41.333	28.529	16.642		17.53	A
	MOTA	1402	CG	TYR A		40.013	28.362	15.927		19.32	A
	MOTA	1403		TYR A		38.859	28.010	16.625		17.69	A
35	MOTA	1404		TYR A		37.617	27.976	15.990		18.18	A
	ATOM	1405		TYR A		39.897	28.664	14.569		16.87	A
	ATOM	1406	CE2	TYR A	248	38.665	28.635	13.924	1.00	19.17	A
	MOTA	1407	CZ	TYR A	248	37.527	28.295	14.643	1.00	19.46	A
	MOTA	1408	OH	TYR A	248	36.299	28.311	14.023	1.00	18.98	A
40	ATOM	1409	C	TYR A	248	42.810	30.039	17.993	1.00	20.42	A
	ATOM	1410	0	TYR A	248	43.208	29.191	18.792	1.00	19.19	A
	ATOM	1411	N	VAL A		43.523	31.114	17.673		20.20	A
	ATOM	1412	CA	VAL A		44.841	31.343	18.251		20.91	A
	ATOM	1413	CB	VAL A		45.542	32.532	17.570		21.18	A
45	ATOM	1414		VAL A		46.821	32.896	18.317		22.45	A
43											
	ATOM	1415		VAL A		45.862	32.170	16.139		24.01	A
	MOTA	1416	С	VAL A		44.764	31.606	19.750		21.52	A
	MOTA	1417	0	VAL A		43.915	32.368	20.216		22.72	A
	MOTA	1418	N	SER A		45.654	30.965	20.503		20.70	A
50	MOTA	1419	CA	SER A		45.697	31.133	21.951		21.65	A
	MOTA	1420	CB	SER A	250	46.370	29.919	22.613	1.00	22.02	A
	MOTA	1421	OG	SER A	250	47.692	29.725	22.132	1.00	22.12	A
	ATOM	1422	C	SER A	250	46.476	32.402	22.280	1.00	22.13	A
	ATOM	1423	0	SER A	250	47.332	32.828	21.511	1.00	22.77	A
55	MOTA	1424	N	PRO A		46.180	33.029	23.425		22.23	A
	ATOM	1425	CD	PRO A		45.163	32.684	24.433		22.97	A
	ATOM	1426	CA	PRO A		46.893	34.254	23.800		22.52	A
	ATOM	1427	CB	PRO A		46.233	34.650	25.127		23.06	A
	ATOM	1428	CG	PRO A		45.726	33.329	25.676		22.55	A
	ATOM	1470	-6	LINU A	231	13.120	55.569	23.070	1.00	22.33	м

	ATOM	1429	С	PRO	-	251	48.414	34.115	23.907	1 00	22.15	A
	MOTA	1430	0	PRO			49.143	35.047	23.563		22.62	A
	MOTA	1431	N	GLU			48.901	32.966	24.367		20.69	A
	ATOM	1432	CA	GLU	Α	252	50.347	32.772	24.500	1.00	21.40	A
5	ATOM	1433	CB	GLU	Α	252	50.673	31.382	25.071	1.00	20.59	A
	ATOM	1434	CG	GLU			49.993	30.232	24.352	1.00	21.91	A
	ATOM	1435	CD	GLU			48.691	29.822	25.014		21.51	A
	ATOM	1436		GLU			47.989	30.707	25.550		21.46	
												A
	MOTA	1437		GLU			48.367	28.613	24.993		20.23	A
10	MOTA	1438	C	GLU			51.071	32.970	23.167		22.99	A
	MOTA	1439	0	GLU			52.191	33.480	23.136		23.17	A
	ATOM	1440	N	LEU	Α	253	50.441	32.576	22.064	1.00	23.00	A
	MOTA	1441	CA	LEU	Α	253	51.068	32.753	20.758	1.00	25.62	A
	ATOM	1442	CB	LEU	Α	253	50.277	32.029	19.669	1.00	26.75	A
15	ATOM	1443	CG	LEU	А	253	50.743	30.620	19.296	1.00	31.87	A
	ATOM	1444		LEU			50.433	29.651	20.422		31.81	A
	ATOM	1445		LEU			50.044	30.179	18.015		31.86	A
	ATOM	1446	C	LEU			51.201	34.228	20.371		26.94	A
	MOTA	1447	0	LEU			52.107	34.601	19.626		27.09	A
20	MOTA	1448	N	LEU			50.297	35.059	20.877		25.83	A
	ATOM	1449	CA	LEU			50.297	36.485	20.564		27.26	A
	MOTA	1450	CB	LEU	Α	254	48.858	37.006	20.564	1.00	25.84	A
	ATOM	1451	CG	LEU	Α	254	47.882	36.290	19.621	1.00	24.69	A
	ATOM	1452	CD1	LEU	Α	254	46.459	36.724	19.932	1.00	23.64	A
25	ATOM	1453		LEU			48.236	36.597	18.177		24.24	A
	ATOM	1454	C	LEU			51.134	37.314	21.537		30.62	A
	ATOM	1455	ō	LEU			51.633	38.383	21.187		32.35	A
	MOTA	1456	N	THR			51.292	36.821	22.758		32.47	A
	MOTA	1457	CA	THR			52.056	37.547	23.759		36.70	A
30	ATOM	1458	CB	THR			51.368	37.478	25.127		34.51	A
	MOTA	1459		THR			51.188	36.106	25.494	1.00	35.49	A
	ATOM	1460	CG2	THR	Α	255	50.013	38.166	25.077	1.00	33.40	A
	ATOM	1461	С	THR	Α	255	53.477	37.035	23.910	1.00	40.09	A
	ATOM	1462	0	THR			54.430	37.793	23.772		43.69	A
35	ATOM	1463	N	GLU			53.617	35.747	24.189		44.77	A
	ATOM	1464	CA	GLU			54.932	35.144	24.382		49.15	A
	ATOM	1465	CB	GLU			54.866	34.143	25.534		51.24	A
	ATOM	1466	CG	GLU			54.514	34.786	26.862		56.03	A
	MOTA	1467	CD	GLU			54.053	33.780	27.893		58.83	A
40	MOTA	1468		GLU			54.766	32.776	28.107		62.13	A
	ATOM	1469		GLU			52.979	33.996	28.494		60.34	A
	MOTA	1470	C	GLU	Α	256	55.475	34.456	23.137	1.00	50.09	A
	ATOM	1471	0	GLU	Α	256	56.616	33.995	23.127	1.00	50.42	A
	ATOM	1472	N	LYS	Α	257	54.658	34.389	22.090	1.00	51.21	A
45	ATOM	1473	CA	LYS			55.064	33.746	20.845	1.00	51.22	A
	ATOM	1474	CB	LYS			56.244	34.502	20.227		53.28	A
	ATOM	1475	CG	LYS			56.558	34.125	18.790		55.19	A
	ATOM	1476	CD	LYS			57.709	34.961	18.253		57.52	A
	ATOM	1477	CE	LYS			57.952	34.694	16.777		58.52	A
50	MOTA	1478	NZ	LYS			58.290	33.268	16.515		60.88	A
	MOTA	1479	C	LYS	Α	257	55.467	32.302	21.138	1.00	50.74	A
	MOTA	1480	0	LYS	Α	257	56.432	31.790	20.577	1.00	52.26	A
	ATOM	1481	N	SER	Α	258	54.721	31.654	22.027	1.00	48.07	A
	ATOM	1482	CA	SER			54.999	30.273	22.402		46.87	A
55	ATOM	1483	CB	SER			55.590	30.229	23.812		48.88	A
	ATOM	1484	OG	SER			54.741	30.892	24.734		53.14	A
	ATOM	1485	C	SER			53.735	29.415	22.342		44.07	A
			0									
	MOTA	1486		SER			52.617	29.932	22.417		44.17	A
	MOTA	1487	N	ALA	A	259	53.917	28.105	22.204	1.00	38.30	A

	ATOM	1488	CA	ALA	Α	259	52.793	27.180	22.127	1.00	34.73	A
	ATOM	1489	CB	ALA	Α	259	52.551	26.779	20.684	1.00	34.16	A
	MOTA	1490	C	ALA	Α	259	53.042	25.940	22.977	1.00	32.34	A
	ATOM	1491	0	ALA	Α	259	54.172	25.459	23.086	1.00	31.81	A
5	ATOM	1492	N	CYS	Α	260	51.975	25.428	23.579	1.00	28.58	A
	MOTA	1493	CA	CYS	Α	260	52.056	24.244	24.425	1.00	26.27	A
	ATOM	1494	CB	CYS	Α	260	52.183	24.654	25.892	1.00	26.53	A
	ATOM	1495	SG	CYS	Α	260	50.846	25.739	26.469	1.00	32.91	A
	ATOM	1496	С	CYS	Α	260	50.786	23.435	24.224	1.00	22.83	A
10	ATOM	1497	0	CYS	Α	260	49.892	23.856	23.495	1.00	22.14	A
	MOTA	1498	N	LYS	А	261	50.706	22.277	24.868	1.00	20.02	A
	ATOM	1499	CA			261	49.526	21.434	24.744		20.65	A
	ATOM	1500	CB	LYS	Α	261	49.619	20.243	25.696	1.00	23.28	A
	ATOM	1501	CG	LYS	Α	261	50.716	19.253	25.347	1.00	27.44	A
15	ATOM	1502	CD	LYS	Α	261	50.732	18.117	26.350	1.00	29.98	A
	ATOM	1503	CE	LYS	Α	261	51.922	17.203	26.134	1.00	32.34	A
	MOTA	1504	NZ	LYS	А	261	51.940	16.121	27.153	1.00	33.28	A
	ATOM	1505	C			261	48.268	22.229	25.062		19.20	A
	ATOM	1506	0			261	47.253	22.092	24.387		18.08	A
20	ATOM	1507	N	SER	Α	262	48.358	23.068	26.089	1.00	16.92	A
	ATOM	1508	CA	SER	А	262	47.235	23.883	26.534	1.00	18.13	A
	MOTA	1509	CB	SER	Α	262	47.644	24.698	27.770	1.00	18.27	A
	ATOM	1510	OG	SER	Α	262	46.517	25.258	28.421	1.00	22.53	A
	ATOM	1511	С	SER	Α	262	46.736	24.811	25.424	1.00	16.77	A
25	ATOM	1512	0	SER	Α	262	45.591	25.254	25.450	1.00	15.69	A
	ATOM	1513	N			263	47.595	25.118	24.456	1.00	16.44	A
	ATOM	1514	CA	SER	Α	263	47.175	25.970	23.347	1.00	16.89	A
	ATOM	1515	CB	SER	Α	263	48.340	26.228	22.382	1.00	18.49	A
	MOTA	1516	OG	SER	Α	263	49.402	26.909	23.031	1.00	22.10	A
30	MOTA	1517	C	SER	Α	263	46.040	25.257	22.612	1.00	17.79	A
	ATOM	1518	0	SER	Α	263	45.099	25.898	22.148	1.00	17.57	A
	ATOM	1519	N	ASP	Α	264	46.119	23.928	22.517	1.00	16.30	A
	MOTA	1520	CA	ASP	Α	264	45.069	23.166	21.836	1.00	16.72	A
	ATOM	1521	CB	ASP	Α	264	45.483	21.704	21.620	1.00	15.92	A
35	ATOM	1522	CG	ASP	Α	264	46.544	21.539	20.548	1.00	17.93	A
	ATOM	1523	OD1	ASP	Α	264	46.642	22.412	19.661	1.00	16.78	A
	ATOM	1524	OD2	ASP	Α	264	47.265	20.515	20.579	1.00	16.64	A
	MOTA	1525	C	ASP			43.773	23.194	22.646	1.00	17.67	A
	MOTA	1526	0	ASP	Α	264	42.681	23.197	22.076	1.00	18.27	A
40	MOTA	1527	N	LEU	Α	265	43.898	23.205	23.974	1.00	15.49	A
	MOTA	1528	CA	LEU	Α	265	42.730	23.232	24.849	1.00	14.75	A
	MOTA	1529	CB	LEU	Α	265	43.147	23.038	26.313	1.00	11.38	A
	MOTA	1530	CG	LEU	Α	265	43.711	21.641	26.621	1.00	14.04	A
	MOTA	1531	CD1	LEU	Α	265	44.249	21.579	28.052	1.00	13.96	A
45	ATOM	1532	CD2	LEU	Α	265	42.619	20.603	26.416	1.00	11.62	A
	MOTA	1533	C	LEU	Α	265	41.999	24.557	24.675	1.00	15.13	A
	MOTA	1534	0	LEU	Α	265	40.777	24.620	24.785	1.00	16.75	A
	MOTA	1535	N	TRP	Α	266	42.746	25.622	24.405	1.00	16.08	A
	MOTA	1536	CA	TRP	Α	266	42.118	26.918	24.184	1.00	16.96	A
50	MOTA	1537	CB	TRP	Α	266	43.176	28.015	24.023	1.00	17.28	A
	MOTA	1538	CG	TRP	Α	266	42.618	29.326	23.521	1.00	20.54	A
	MOTA	1539	CD2	TRP	Α	266	42.313	30.490	24.301	1.00	20.07	A
	ATOM	1540	CE2	TRP	Α	266	41.782	31.459	23.417	1.00	20.46	A
	MOTA	1541	CE3	TRP			42.435	30.810	25.660		20.68	A
55	MOTA	1542		TRP			42.270	29.631	22.231		19.53	A
	MOTA	1543	NE1				41.769	30.908	22.163		19.61	A
	MOTA	1544	CZ2	TRP			41.372	32.727	23.850	1.00	20.90	A
	MOTA	1545	CZ3				42.026	32.073	26.091		19.45	A
	ATOM	1546	CH2	TRP	Α	266	41.501	33.015	25.185	1.00	20.71	A

	ATOM	1547	C	TRP	Α	266	41.284	26.795	22.913	1.00	17.22	A
	ATOM	1548	0	TRP	Δ	266	40.139	27.240	22.863	1.00	18 03	A
	MOTA	1549	N	ALA			41.863	26.181	21.886		17.50	A
	ATOM	1550	CA	ALA	Α	267	41.155	25.990	20.626	1.00	16.16	A
5	ATOM	1551	CB	ALA			42.050	25.290	19.621	1.00		А
,												
	MOTA	1552	C	ALA	Α	267	39.901	25.159	20.891	1.00	16.28	A
	ATOM	1553	0	ALA	А	267	38.835	25.436	20.346	1.00	16.46	A
	MOTA	1554	N	LEU			40.031	24.144	21.739	1.00		A
	ATOM	1555	CA	LEU	Α	268	38.890	23.299	22.084	1.00	17.03	A
10	ATOM	1556	CB	LEU	A	268	39.292	22.260	23.139	1.00	15.35	A
	ATOM	1557	CG	LEU				21.429	23.754	1.00		A
							38.158					
	ATOM	1558	CD1	LEU	Α	268	37.505	20.578	22.678	1.00	16.17	A
	ATOM	1559	CD2	LEU	A	268	38.718	20.537	24.881	1.00	17.49	A
	ATOM	1560	C	LEU			37.766	24.179	22.628	1.00		A
15	ATOM	1561	0	LEU	Α	268	36.603	24.031	22.247	1.00	15.28	A
	ATOM	1562	N	GLY	А	269	38.119	25.099	23.520	1.00	14.34	A
	ATOM	1563	CA	GLY			37.124	25,989	24.092	1.00		A
	ATOM	1564	C	GLY	Α	269	36.406	26.808	23.031	1.00	14.94	A
	ATOM	1565	0	GLY	А	269	35.193	27.014	23.114	1.00	14.76	A
20	ATOM	1566	N	CYS			37.146	27.279	22.030	1.00		A
20												
	ATOM	1567	CA	CYS	А	270	36.539	28.061	20.958	1.00	16.80	A
	ATOM	1568	CB	CYS	А	270	37.611	28.634	20.023	1.00	15.97	A
	ATOM	1569	SG	CYS			38.751	29.810	20.780	1.00		A
	MOTA	1570	С	CYS			35.598	27.175	20.140	1.00		A
25	ATOM	1571	0	CYS	Α	270	34.516	27.604	19.741	1.00	18.38	A
	ATOM	1572	N	ILE	Δ	271	36.022	25.939	19.887	1 00	16.99	A
	ATOM	1573	CA	ILE			35.221	25.004	19.104	1.00		A
	ATOM	1574	CB	ILE	Α	271	36.038	23.741	18.778	1.00	16.53	A.
	ATOM	1575	CG2	ILE	А	271	35.155	22.694	18.102	1.00	16.34	A
30	ATOM	1576					37.222	24.129	17.882		15.59	A
50												
	MOTA	1577	CDI	ILE			38.239	23.018	17.690	1.00		A
	ATOM	1578	C	ILE	Α	271	33.920	24.626	19.809	1.00	16.74	A
	ATOM	1579	0	ILE	Δ	271	32.865	24.576	19.179	1.00	17.12	A
	ATOM	1580	N	ILE			33.990	24.357	21.111	1.00		A
35	ATOM	1581	CA	ILE	Α	272	32.785	24.021	21.862	1.00	18.30	A.
	ATOM	1582	CB	ILE	А	272	33.097	23.747	23.346	1.00	17.77	A
	ATOM	1583		ILE			31.796	23.666	24.152	1.00		A
	MOTA	1584		ILE			33.877	22.437	23.481	1.00		A
	ATOM	1585	CD1	ILE	A	272	34.446	22.217	24.886	1.00	18.64	A
40	ATOM	1586	C	ILE	Δ	272	31.824	25.207	21.776	1.00	19 51	A
	MOTA	1587	0	ILE			30.624	25.037	21.554	1.00		A.
	MOTA	1588	N	TYR	Α	273	32.362	26.409	21.947	1.00	18.52	A
	ATOM	1589	CA	TYR	A	27.3	31.553	27.615	21.881	1.00	20.48	A
	ATOM	1590	CB	TYR			32.418	28.847	22.162	1.00		A
45	ATOM	1591	CG	TYR	Α	273	31.663	30.161	22.125	1.00	20.26	A
	ATOM	1592	CD1	TYR	А	273	31.229	30.709	20.916	1.00	20.67	A
	ATOM	1593		TYR			30.536	31.917	20.880	1.00		A
	ATOM	1594	CD2	TYR	A	273	31.383	30.857	23.302	1.00	19.82	A
	ATOM	1595	CE2	TYR	Α	273	30.691	32.062	23.280	1.00	20.62	A
50	ATOM	1596	CZ	TYR	Δ	273	30.271	32.587	22.067	1.00	21 15	A
50												
	MOTA	1597	OH	TYR			29.588	33.776	22.049	1.00		A
	ATOM	1598	C	TYR	A	273	30.902	27.730	20.507	1.00	21.54	A
	ATOM	1599	0	TYR			29.719	28.049	20.401	1.00		A
	ATOM	1600	N	GLN			31.676	27.454	19.461	1.00		A
55	MOTA	1601	CA	GLN	Α	274	31.176	27.538	18.095	1.00	21.48	A
	ATOM	1602	CB	GLN	Α	274	32.323	27.341	17.097	1.00	21.41	A
	ATOM	1603	CG	GLN			31.934	27.596	15.645	1.00		A
	ATOM	1604	CD	GLN			33.131	27.588	14.706	1.00		A
	MOTA	1605	OE1	GLN	Α	274	34.276	27.446	15.139	1.00	22.51	A

	ATOM	1606	ME 2	GLN	70	274	32.870	27.750	13.413	1 00	22.96	A
	MOTA	1607	С	GLN			30.076	26.517	17.828		21.51	A
	MOTA	1608	0	GLN			29.123	26.806	17.108		20.50	A
	ATOM	1609	N	LEU	Α	275	30.207	25.324	18.403	1.00	21.44	A
5	ATOM	1610	CA	LEU	Α	275	29.196	24.282	18.208	1.00	20.95	A
	ATOM	1611	CB	LEU	Α	275	29.645	22.958	18.846	1.00	19.11	A
	ATOM	1612	CG	LEU			30.775	22.182	18.159		21.43	A
	ATOM	1613		LEU			31.118	20.936	18.963		17.64	A
10	ATOM	1614		LEU			30.342	21.795	16.754		20.34	A
10	MOTA	1615	С	LEU			27.860	24.697	18.815		21.32	A
	MOTA	1616	0	LEU			26.802	24.461	18.229		19.75	A
	MOTA	1617	N	VAL	Α	276	27.921	25.322	19.987	1.00	19.10	A
	ATOM	1618	CA	VAL	Α	276	26.724	25.750	20.702	1.00	22.47	A
	ATOM	1619	CB	VAL	Α	276	27.011	25.882	22.217	1.00	20.87	A
15	ATOM	1620	CG1	VAL	Α	276	25.742	26.291	22.957	1.00	19.68	A
	ATOM	1621		VAL			27.550	24.558	22.766		19.43	A
	ATOM	1622	c	VAL			26.127	27.075	20.211		23.89	A
	ATOM	1623	o	VAL			24.910	27.199	20.211		24.90	A
	MOTA	1624	N	ALA			26.983	28.062	19.965		24.56	A
20	MOTA	1625	CA	ALA			26.533	29.374	19.518		24.72	A
	MOTA	1626	CB	ALA	Α	277	27.504	30.444	19.999	1.00	24.36	A
	MOTA	1627	C	ALA	Α	277	26.378	29.458	18.005	1.00	25.76	A
	ATOM	1628	0	ALA	Α	277	25.577	30.242	17.502	1.00	26.39	A
	ATOM	1629	N	GLY	Α	278	27.142	28.651	17.280	1.00	25.13	A
25	ATOM	1630	CA	GLY			27.062	28.673	15.834		25.58	A
20	ATOM	1631	C	GLY			28.163	29.524	15.231		26.50	A
			o	GLY			28.374	29.510	14.015		28.17	
	MOTA	1632										A
	ATOM	1633	N	LEU			28.866	30.262	16.086		24.44	A
	MOTA	1634	CA	LEU			29.962	31.130	15.656		25.21	A
30	MOTA	1635	CB	LEU			29.468	32.575	15.500		25.78	A
	ATOM	1636	CG	LEU	Α	279	28.364	32.899	14.490	1.00	28.17	A
	ATOM	1637	CD1	LEU	Α	279	27.922	34.344	14.684	1.00	26.60	A
	ATOM	1638	CD2	LEU	Α	279	28.862	32.670	13.071	1.00	26.52	A
	ATOM	1639	С	LEU			31.093	31.116	16.687		23.47	A
35	ATOM	1640	ō	LEU			30.848	30.994	17.882		24.44	A
33	ATOM	1641	N	PRO			32.349	31.239	16.236		23.35	A
	MOTA	1642	CD	PRO			32.831	31.404	14.855		22.26	A
	MOTA	1643	CA	PRO			33.464	31.239	17.189		23.81	A
	MOTA	1644	CB	PRO			34.692	31.293	16.282		23.24	A
40	MOTA	1645	CG	PRO			34.189	32.020	15.073		24.89	A
	ATOM	1646	C	PRO	Α	280	33.353	32.444	18.137	1.00	22.69	A
	ATOM	1647	0	PRO	Α	280	32.750	33.457	17.788	1.00	22.11	A
	ATOM	1648	N	PRO	Α	281	33.939	32.344	19.345	1.00	23.06	A
	ATOM	1649	CD	PRO	А	281	34.810	31.223	19.734	1.00	21.37	A
45	ATOM	1650	CA	PRO			33.935	33.375	20.395		23.67	A
75	ATOM	1651	CB	PRO			34.781	32.751	21.509		24.89	A
	ATOM	1652	CG	PRO			34.749	31.287	21.219		25.24	A
	MOTA	1653	С	PRO			34.481	34.752	20.017		23.75	A
	MOTA	1654	0	PRO			33.869	35.781	20.317		21.02	A
50	MOTA	1655	N	PHE	А	282	35.644	34.763	19.379	1.00	22.17	A
	ATOM	1656	CA	PHE	Α	282	36.293	36.007	18.998	1.00	23.16	A
	MOTA	1657	CB	PHE	Α	282	37.765	35.943	19.406	1.00	21.01	A
	ATOM	1658	CG	PHE			37.975	35.482	20.822		22.66	A
	ATOM	1659		PHE			37.806	36.361	21.888		20.06	A
55	ATOM	1660	CD2	PHE			38.291	34.151	21.093		20.72	A
55			CE1									
	ATOM	1661		PHE			37.947	35.921	23.206		22.66	A
	MOTA	1662	CE2	PHE			38.433	33.702	22.405		20.97	A
	MOTA	1663	CZ	PHE			38.261	34.590	23.466		19.58	A
	MOTA	1664	C	PHE	Α	282	36.169	36.263	17.503	1.00	24.39	A

	ATOM	1665	0	PHE	2	202	36.802	35.585	16.694	1 00	25.80	A
	MOTA	1666	N	ARG			35.355	37.248	17.142		24.99	A
	MOTA	1667	CA	ARG			35.141	37.594	15.741		26.33	A
	MOTA	1668	CB	ARG	Α	283	33.721	37.209	15.316	1.00	28.91	A
5	ATOM	1669	CG	ARG	А	283	33.293	35.808	15.724	1.00	30.27	A
	MOTA	1670	CD	ARG	A	283	31.904	35.493	15.188	1.00	33.36	A
	ATOM	1671	NE	ARG			30.890	36.392	15.733		32.76	A
	ATOM	1672	CZ	ARG			30.372	36.287	16.952		34.79	A
10	ATOM	1673		ARG			30.767	35.317	17.768		35.77	A
10	MOTA	1674		ARG			29.458	37.156	17.359		36.12	A
	MOTA	1675	C	ARG			35.328	39.096	15.544		26.47	A
	ATOM	1676	0	ARG			35.029	39.888	16.438		26.28	A
	MOTA	1677	N	ALA	Α	284	35.818	39.486	14.373	1.00	26.70	A
	ATOM	1678	CA	ALA	Α	284	36.033	40.899	14.079	1.00	27.84	A
15	ATOM	1679	CB	ALA	Α	284	37.188	41.442	14.914	1.00	26.24	A
	ATOM	1680	С	ALA	А	284	36.327	41.077	12.602	1.00	28.35	A
	ATOM	1681	Ó	ALA			36.560	40.101	11.891		29.91	A
	ATOM	1682	N	GLY			36.332	42.329	12.153		29.29	A
	ATOM	1683	CA	GLY			36.577	42.631	10.753		29.52	A
20												
20	ATOM	1684	C	GLY			37.893	42.156	10.168		30.12	A
	MOTA	1685	0	GLY			37.974	41.862	8.976		30.60	A
	MOTA	1686	N	ASN			38.939	42.097	10.983		28.49	A
	MOTA	1687	CA	ASN	Α	286	40.231	41.644	10.489	1.00	26.71	A
	ATOM	1688	CB	ASN	Α	286	41.050	42.825	9.945	1.00	26.11	A
25	ATOM	1689	CG	ASN	Α	286	41.310	43.900	10.990	1.00	27.83	A
	ATOM	1690	OD1	ASN	А	286	41.877	43.631	12.049	1.00	27.84	A
	ATOM	1691		ASN			40.908	45.131	10.685		25.95	A
	ATOM	1692	C	ASN			40.997	40.924	11.584		26.03	A
	ATOM	1693	o	ASN			40.540	40.851	12.723		25.66	A
30				GLU								
30	ATOM	1694	N				42.162	40.391	11.239		24.81	A
	MOTA	1695	CA	GLU			42.965	39.662	12.206		27.59	A
	MOTA	1696	CB	GLU			44.145	38.985	11.510		30.17	A
	MOTA	1697	CG	GLU			43.776	37.632	10.931		38.21	A
	MOTA	1698	CD	GLU	Α	287	44.900	36.998	10.140	1.00	41.86	A
35	ATOM	1699	OE1	GLU	Α	287	46.061	37.036	10.608	1.00	43.08	A
	ATOM	1700	OE2	GLU	Α	287	44.612	36.449	9.052	1.00	45.22	A
	ATOM	1701	С	GLU	Α	287	43.459	40.485	13.383	1.00	25.05	A
	ATOM	1702	0	GLU			43.382	40.030	14.521		26.41	A
	ATOM	1703	N	TYR			43.966	41.685	13.122		23.04	A
40	ATOM	1704	CA	TYR			44.460	42.528	14.205		22.34	A
40	ATOM	1705	CB	TYR			44.867	43.913	13.691		21.07	A
				TYR					14.805		21.07	
	ATOM	1706	CG				45.275	44.858				A
	ATOM	1707		TYR			46.533	44.762	15.405		21.23	A
	ATOM	1708		TYR			46.891	45.588	16.475		20.43	A
45	MOTA	1709		TYR			44.380	45.809	15.302		22.32	A
	MOTA	1710	CE2	TYR	Α	288	44.725	46.637	16.373	1.00	23.28	A
	MOTA	1711	CZ	TYR	Α	288	45.981	46.518	16.953	1.00	22.96	A
	MOTA	1712	OH	TYR	Α	288	46.316	47.313	18.024	1.00	23.18	A
	ATOM	1713	С	TYR			43.402	42.698	15.288		21.38	A
50	ATOM	1714	0	TYR			43.710	42.616	16.473		22.09	A
50	ATOM	1715	N	LEU			42.159	42.939	14.874		21.88	A
	ATOM	1716	CA	LEU			41.055	43.130	15.811		21.98	A
	ATOM	1717	CB	LEU			39.821	43.673	15.078		22.90	A
	MOTA	1718	CG	LEU			39.896	45.130	14.601		26.52	A
55	MOTA	1719		LEU			38.706	45.436	13.696		26.55	A
	MOTA	1720		LEU			39.914	46.071	15.807		23.13	A
	MOTA	1721	C	LEU	Α	289	40.686	41.849	16.560	1.00	21.24	A
	MOTA	1722	0	LEU	Α	289	40.256	41.897	17.715	1.00	20.72	A
	MOTA	1723	N	ILE	Α	290	40.843	40.708	15.900	1.00	19.62	A

	3.0001	1704		TT 17		000	40 530	20 422	16 533	1 00 1		-
	MOTA	1724	CA			290	40.538	39.433	16.533	1.00 1		Α
	MOTA	1725	CB	ILE	А	290	40.560	38.281	15.509	1.00 1		Α
	ATOM	1726	CG2	ILE	Α	290	40.503	36.934	16.234	1.00 1	7.63	Α
	ATOM	1727	CG1	ILE	Δ	290	39.378	38.429	14.545	1.00 1	8 8 8	Α
5												
3	MOTA	1728		ILE			39.421	37.483	13.357	1.00 1		А
	MOTA	1729	C	ILE	Α	290	41.578	39.167	17.618	1.00 1	9.09	Α
	ATOM	1730	0	ILE	Α	290	41.236	38.788	18.737	1.00 1	3.20	Α
	ATOM	1731	N	DHE	75	291	42.849	39.376	17.286	1.00 18	76	Α
		1732	CA									
	ATOM					291	43.925	39.156	18.247	1.00 20		А
10	MOTA	1733	CB			291	45.286	39.434	17.606	1.00 20		А
	ATOM	1734	CG	PHE	А	291	45.644	38.480	16.503	1.00 23	2.92	Α
	ATOM	1735	CD1	PHE	Δ	291	45.065	37.214	16.443	1.00 2	2.98	Α
	ATOM	1736		PHE			46.588	38.830	15.543	1.00 2		A
	ATOM	1737		PHE			45.423	36.310	15.440	1.00 2		Α
15	MOTA	1738	CE2	PHE	Α	291	46.954	37.931	14.535	1.00 2	5.54	Α
	ATOM	1739	CZ	PHE	А	291	46.370	36.670	14.485	1.00 2	3.29	Α
	ATOM	1740	С	DHE	70.	291	43.739	40.061	19.451	1.00 2	1 72	А
	ATOM	1741	ō			291	43.992	39.671	20.593	1.00 2		Α
	ATOM	1742	N			292	43.284	41.275	19.178	1.00 2		Α
20	MOTA	1743	CA	GLN	Α	292	43.055	42.264	20.216	1.00 2	4.01	A
	ATOM	1744	CB	GLN	Α	292	42.574	43.559	19.562	1.00 2	5.77	Α
	ATOM	1745	CG			292	42.577	44.773	20.447	1.00 2		Α
	ATOM	1746	CD			292	42.469	46.057	19.638	1.00 2		Α
	ATOM	1747	OE1	GLN	Α	292	41.520	46.244	18.872	1.00 2	7.16	А
25	ATOM	1748	NE2	GLN	Α	292	43.449	46.944	19.799	1.00 2	7.61	Α
	ATOM	1749	C	GT.N	A	292	42.018	41.733	21.204	1.00 23	2.97	Α
	ATOM	1750	o			292	42.200	41.832	22.415	1.00 2		Α
	MOTA	1751	N			293	40.937	41.154	20.687	1.00 2		А
	ATOM	1752	CA	LYS			39.895	40.612	21.558	1.00 2		Α
30	MOTA	1753	CB	LYS	Α	293	38.664	40.223	20.740	1.00 23	2.69	Α
	ATOM	1754	CG	LYS	А	293	37.919	41.407	20.153	1.00 2	5.78	А
	ATOM	1755	CD	LYS			36.651	40.961	19.429	1.00 2		A
	MOTA	1756	CE	LYS			35.857	42.161	18.926	1.00 30		А
	MOTA	1757	NZ	LYS	Α	293	34.612	41.750	18.214	1.00 3	2.98	Α
35	ATOM	1758	C	LYS	Α	293	40.398	39.398	22.343	1.00 2	1.20	Α
	ATOM	1759	0	LYS	А	293	40.041	39.204	23.509	1.00 2	2.01	А
	ATOM	1760	N			294	41.226	38.583	21.702	1.00 1		A
	MOTA	1761	CA			294	41.774	37.394	22.347	1.00 20		Α
	MOTA	1762	CB	ILE	Α	294	42.631	36.575	21.349	1.00 1	3.98	Α
40	ATOM	1763	CG2	ILE	Α	294	43.481	35.550	22.098	1.00 1	7.70	Α
	ATOM	1764	CG1	ILE	А	294	41.716	35.897	20.318	1.00 1	7.93	А
	ATOM	1765		ILE			42.467	35.237	19.178	1.00 1		A
	ATOM	1766	C			294	42.618	37.727	23.587	1.00 2		Α
	MOTA	1767	0	ILE	Α	294	42.366	37.199	24.673	1.00 20	0.86	Α
45	ATOM	1768	N	ILE	Α	295	43.610	38.600	23.439	1.00 2	1.88	Α
	ATOM	1769	CA	TLE	A	295	44.461	38.934	24.582	1.00 2	4.25	А
	ATOM	1770	CB			295	45.668	39.805	24.175	1.00 2		A
	MOTA	1771		ILE			46.514	39.066	23.140	1.00 2		Α
	MOTA	1772	CG1	ILE	Α	295	45.189	41.151	23.637	1.00 2	4.58	Α
50	ATOM	1773	CD1	ILE	Α	295	46.317	42.149	23.433	1.00 2	6.69	A
	ATOM	1774	С	TLE	Α	295	43.720	39.636	25.717	1.00 2	4.80	А
			ō							1.00 2		
	ATOM	1775				295	44.214	39.687	26.842			Α
	MOTA	1776	N			296	42.539	40.173	25.425	1.00 2		Α
	MOTA	1777	CA	LYS	Α	296	41.743	40.853	26.444	1.00 2	6.80	Α
55	ATOM	1778	CB	LYS	Α	296	41.178	42.170	25.894	1.00 2	7.39	Α
	ATOM	1779	CG	LYS			42.240	43.141	25.413	1.00 3		Α
	ATOM	1780	CD			296	41.634	44.410	24.826	1.00 3		A
	MOTA	1781	CE			296	41.009	45.283	25.900	1.00 3		Α
	MOTA	1782	NZ	LYS	Α	296	40.564	46.603	25.357	1.00 4	1.72	Α

	ATOM	1783	C	LYS			40.593	39.958	26.893		25.50	A
	ATOM	1784	0	LYS	Α	296	39.770	40.361	27.713	1.00	24.02	A
	ATOM	1785	N	LEU	Α	297	40.550	38.742	26.349	1.00	25.67	Α
	ATOM	1786	CA	LEU			39.500	37.777	26.666		25.16	A
_												
5	MOTA	1787	CB	LEU			39.632	37.285	28.111		24.80	A
	ATOM	1788	CG	LEU	Α	297	38.766	36.068	28.460	1.00	26.43	A
	MOTA	1789	CD1	LEU	А	297	39.238	34.852	27.646	1.00	26.70	A
	ATOM	1790		LEU			38.856	35.777	29.951		24.84	A
				LEU								
	MOTA	1791	C				38.151	38.459	26.467		25.11	A
10	MOTA	1792	0	LEU			37.261	38.378	27.309		25.28	A
	MOTA	1793	N	GLU	Α	298	38.007	39.127	25.331	1.00	24.98	A.
	ATOM	1794	CA	GLU	Α	298	36.786	39.847	25.023	1.00	25.31	A
	ATOM	1795	CB	GLU			37.143	41.139	24.291		27.13	A
	ATOM	1796	CG	GLU			35.991	42.092	24.108		31.28	A
15	MOTA	1797	CD	GLU			36.419	43.362	23.410		34.40	A
	MOTA	1798		GLU			37.348	44.027	23.918	1.00	35.90	A
	ATOM	1799	OE2	GLU	Α	298	35.832	43.693	22.359	1.00	36.16	A
	ATOM	1800	C	GLU	Α	298	35.766	39.057	24.207	1.00	23.79	A
	ATOM	1801	0	GLU	Δ	298	35.832	39.017	22.979	1 00	24.35	A
20	ATOM	1802	N	TYR			34.825	38.427	24.902		23.45	A
20												
	MOTA	1803	CA	TYR			33.760	37.663	24.265		23.98	A
	MOTA	1804	CB	TYR	Α	299	34.264	36.304	23.755	1.00	20.13	A
	MOTA	1805	CG	TYR	Α	299	34.348	35.233	24.828	1.00	21.17	A
	ATOM	1806	CD1	TYR	А	299	35.336	35.279	25.810	1.00	19.32	A
25	ATOM	1807	CE1	TYR			35.389	34.332	26.826		19.30	A
23												
	MOTA	1808	CD2	TYR			33.410	34.201	24.888		18.96	A
	MOTA	1809	CE2	TYR			33.456	33.243	25.907		19.41	A
	MOTA	1810	CZ	TYR	Α	299	34.449	33.321	26.870	1.00	18.79	A
	ATOM	1811	OH	TYR	Α	299	34.511	32.401	27.881	1.00	18.77	A
30	ATOM	1812	C	TYR			32.699	37.437	25.331		25.20	A
50	ATOM	1813	ŏ	TYR			32.942	37.681	26.506		26.46	A
	MOTA	1814	N	ASP			31.522	36.981	24.927		26.94	A
	MOTA	1815	CA	ASP	Α	300	30.467	36.710	25.891	1.00	30.60	A
	ATOM	1816	CB	ASP	Α	300	29.665	37.981	26.179	1.00	35.86	A
35	ATOM	1817	CG	ASP	А	300	29.228	38.687	24.923	1.00	42.04	A
	ATOM	1818		ASP			28.450	38.088	24.149		45.98	A
	ATOM	1819		ASP			29.666	39.840	24.707		45.69	A
	MOTA	1820	C	ASP			29.564	35.608	25.363		29.26	A
	MOTA	1821	0	ASP	Α	300	29.590	35.299	24.172	1.00	28.64	A
40	MOTA	1822	N	PHE	Α	301	28.778	35.011	26.253	1.00	28.96	A
	ATOM	1823	CA	PHE	A	301	27.884	33.924	25.871	1.00	30.48	A
	ATOM	1824	CB	PHE			27.818	32.854	26.968		29.17	A
	ATOM	1825	CG	PHE			29.147	32.279	27.356		29.29	A
	MOTA	1826		PHE			29.978	32.949	28.245		27.31	A
45	MOTA	1827	CD2	PHE	Α	301	29.560	31.050	26.845	1.00	27.89	A
	ATOM	1828	CE1	PHE	Α	301	31.205	32.403	28.625	1.00	28.83	A
	ATOM	1829	CE2	PHE	Δ	301	30.781	30.498	27.217	1.00	28.05	A
	ATOM	1830	CZ	PHE			31.605	31.175	28.110		28.27	A
	MOTA	1831	C	PHE			26.459	34.384	25.619		32.20	A
50	MOTA	1832	0	PHE	Α	301	25.946	35.261	26.317	1.00	32.36	A
	MOTA	1833	N	PRO	Α	302	25.798	33.804	24.607	1.00	33.29	A
	MOTA	1834	CD	PRO	Α	302	26.313	32.943	23.529	1.00	34.04	A
	ATOM	1835	CA	PRO			24.415	34.199	24.341		35.24	A
	ATOM	1836		PRO			24.144	33.608	22.959		34.01	A
			CB									
55	MOTA	1837	CG	PRO			25.041	32.413	22.921		35.48	A
	MOTA	1838	C	PRO			23.567	33.561	25.444		37.39	A
	MOTA	1839	0	PRO	Α	302	23.935	32.518	25.986	1.00	38.49	A
	MOTA	1840	N	ALA	Α	303	22.447	34.188	25.783	1.00	39.36	A
	ATOM	1841	CA	ALA			21.572	33.692	26.843		40.65	A
	111 011	1041	J.A.	viny	Λ	505	-1.012	55.052	20.013	1.00	10.00	м

	ATOM	1842	CB	ALA	Α	303	20.280	34.506	26.862	1.00	41.66	A
	ATOM	1843	С	ALA	70	202	21.238	32.197	26.814	1 00	41.25	A
	MOTA	1844	0	ALA			21.253	31.537	27.854		43.16	A
	MOTA	1845	N	ALA	Α	304	20.945	31.665	25.631	1.00	41.04	A
5	ATOM	1846	CA	ALA	Z.	304	20.569	30.258	25.480	1 00	40.66	A
	MOTA	1847	CB	ALA			20.121	30.004	24.040		41.36	A
	ATOM	1848	C	ALA	Α	304	21.628	29.223	25.876	1.00	39.61	A
	ATOM	1849	0	ALA	Δ	304	21.298	28.156	26.395	1 00	40.61	A
	ATOM	1850	N			305	22.891	29.543	25.617		36.21	A
10	MOTA	1851	CA	PHE			24.022	28.662	25.909		32.08	A
	ATOM	1852	CB	PHE	А	305	25.259	29.519	26.187	1.00	29.46	A
	ATOM	1853	CG	PHE	75.	305	26.536	28.917	25.690	1 00	28.15	A
	MOTA	1854		PHE			27.146	27.875	26.377		26.20	A
	ATOM	1855	CD2	PHE	Α	305	27.127	29.386	24.521	1.00	27.05	A
15	ATOM	1856	CE1	PHE	А	305	28.330	27.308	25.908	1.00	26.92	A
	ATOM	1857		PHE			28.312	28.826	24.042		26.62	A
	MOTA	1858	CZ			305	28.914	27.786	24.737		26.61	A
	MOTA	1859	С	PHE	Α	305	23.811	27.664	27.057	1.00	30.09	A
	ATOM	1860	0	PHE	A	305	23.518	28.051	28.187	1.00	31.51	A
20	ATOM	1861	N			306	23.964	26.378	26.758		27.01	A
20												
	ATOM	1862	CA	PHE	А	306	23.801	25.334	27.769	1.00	26.30	A
	ATOM	1863	CB	PHE	Α	306	24.157	23.970	27.170	1.00	25.03	A
	ATOM	1864	CG	PHE			23.548	23.725	25.815		27.24	A
	MOTA	1865		PHE		306	22.170	23.831	25.622		28.40	A
25	ATOM	1866	CD2	PHE	А	306	24.350	23.386	24.728	1.00	27.84	A
	ATOM	1867	CE1	PHE	Α	306	21.601	23.603	24.365	1.00	28.05	A
	ATOM	1868	CE2	PHE	70.	306	23.792	23.155	23.465	1 00	28.31	A
	MOTA	1869	CZ	PHE		306	22.415	23.263	23.283		28.00	A
	ATOM	1870	C	PHE	Α	306	24.711	25.652	28.961	1.00	26.23	A
30	ATOM	1871	0	PHE	А	306	25.927	25.775	28.811	1.00	25.59	A
	ATOM	1872	N	PRO		307	24.125	25.796	30.163		26.67	A
	ATOM	1873	CD	PRO		307	22.685	25.625	30.430		27.95	A
	MOTA	1874	CA	PRO	A	307	24.842	26.110	31.405	1.00	26.59	A
	ATOM	1875	CB	PRO	Δ	307	23.795	25.832	32.481	1 00	26.14	A
35		1876	CG	PRO				26.250			27.86	
33	MOTA						22.531		31.803			A
	ATOM	1877	С	PRO	Α	307	26.145	25.355	31.659	1.00	25.58	A
	MOTA	1878	0	PRO	А	307	27.189	25.964	31.900	1.00	22.65	A
	ATOM	1879	N	LYS			26.085	24.031	31.620		24.46	A
	MOTA	1880	CA	LYS			27.274	23.232	31.867		23.91	A
40	ATOM	1881	CB	LYS	Α	308	26.887	21.760	32.024	1.00	23.25	A
	ATOM	1882	CG	LYS	А	308	26.062	21.532	33.285	1.00	28.49	A
	ATOM	1883	CD	LYS	75	308	25.618	20.093	33.466	1 00	30.17	A
	ATOM	1884	CE	LYS			24.760	19.973	34.722		33.12	A
	ATOM	1885	NZ	LYS	A	308	24.122	18.636	34.860	1.00	34.13	A
45	ATOM	1886	С	LYS	А	308	28.314	23.426	30.769	1.00	22.84	A
	ATOM	1887	0	LYS			29.514	23.411	31.042		22.46	A
	ATOM	1888	N	ALA			27.861	23.621	29.534		21.59	A
	MOTA	1889	CA	ALA	A	309	28.792	23.848	28.432	1.00	20.02	A
	ATOM	1890	CB	ALA	Δ	309	28.056	23.856	27.106	1 00	18.80	A
50								25.191				
30	MOTA	1891	C	ALA			29.481		28.662		21.41	A
	MOTA	1892	0	ALA	Α	309	30.680	25.335	28.427	1.00	21.39	A
	MOTA	1893	N	ARG	A	310	28.717	26.179	29.121	1.00	21.39	A
	ATOM	1894	CA	ARG			29.290	27.494	29.388		22.02	A
	MOTA	1895	CB	ARG			28.213	28.479	29.854		22.39	A
55	MOTA	1896	CG	ARG	Α	310	28.806	29.756	30.436	1.00	25.30	A
	ATOM	1897	CD	ARG	Α	310	27.780	30.852	30.664	1.00	28.33	A
	ATOM	1898	NE	ARG			28.420	32.039	31.230		30.18	A
	MOTA	1899	CZ	ARG			27.901	33.263	31.203		32.07	A
	MOTA	1900	NH1	ARG	Α	310	26.719	33.477	30.634	1.00	31.19	A

	ATOM	1901	MILI 2	ARG	70	210	28.567	34.277	31.742	1 00	30.49	A
		1902	C	ARG			30.376	27.388	30.458		21.65	A
	ATOM							27.300				
	MOTA	1903	0	ARG			31.464		30.311		20.36	A
	MOTA	1904	N	ASP			30.074	26.677	31.541		19.57	A
5	ATOM	1905	CA	ASP		311	31.043	26.512	32.615		20.18	A
	MOTA	1906	CB	ASP	Α	311	30.460	25.649	33.739	1.00	20.39	A
	ATOM	1907	CG	ASP	Α	311	31.439	25.446	34.881	1.00	23.35	A
	ATOM	1908	OD1	ASP	Α	311	32.158	24.428	34.885	1.00	24.91	A
	ATOM	1909	OD2	ASP	Α	311	31.500	26.312	35.776	1.00	26.96	A
10	ATOM	1910	С	ASP	А	311	32.322	25.877	32.073	1.00	19.73	A
	ATOM	1911	Ö	ASP			33.422	26.289	32.439		19.30	A
	ATOM	1912	N	LEU			32.179	24.891	31.188		16.32	A
	ATOM	1913	CA	LEU			33.349	24.226	30.611		16.66	A
	ATOM	1914	CB	LEU			32.927	23.035	29.744		16.12	A A
15												
15	MOTA	1915	CG	LEU			34.050	22.320	28.974		14.73	A
	MOTA	1916		LEU			35.192	21.935	29.912		14.56	A
	MOTA	1917		LEU			33.477	21.084	28.289		14.22	A
	MOTA	1918	С	LEU			34.181	25.189	29.774		16.61	A
	ATOM	1919	0	LEU			35.402	25.241	29.910		16.20	A
20	ATOM	1920	N	VAL	Α	313	33.515	25.949	28.908	1.00	16.20	A
	MOTA	1921	CA	VAL	Α	313	34.207	26.907	28.058	1.00	15.37	A.
	ATOM	1922	CB	VAL	Α	313	33.216	27.648	27.130	1.00	16.42	A
	ATOM	1923	CG1	VAL	Α	313	33.915	28.796	26.426	1.00	16.93	A
	ATOM	1924	CG2	VAL	А	313	32.644	26.672	26.103	1.00	17.88	A
25	ATOM	1925	С	VAL			34.960	27.923	28.911		17.39	A
	ATOM	1926	ō	VAL			36.093	28.294	28.591		18.00	A
	ATOM	1927	N	GLU			34.342	28.364	30.004		17.61	A
	ATOM	1928	CA	GLU		314	34.986	29.331	30.885		20.43	A
				GLU				29.816				
20	ATOM	1929	CB				34.009		31.959		22.14	A
30	ATOM	1930	CG	GLU		314	32.800	30.550	31.396		26.52	A
	MOTA	1931	CD	GLU			31.852	31.025	32.478		31.26	A.
	MOTA	1932		GLU		314	31.580	30.246	33.417		33.48	A
	MOTA	1933		GLU			31.370	32.173	32.387		34.81	A
	MOTA	1934	C	GLU			36.217	28.721	31.539		19.15	A
35	ATOM	1935	0	GLU			37.134	29.433	31.934		21.47	A
	ATOM	1936	N	LYS	Α	315	36.245	27.400	31.651	1.00	19.51	A.
	ATOM	1937	CA	LYS	Α	315	37.394	26.749	32.258	1.00	19.17	A
	ATOM	1938	CB	LYS	Α	315	36.946	25.514	33.043	1.00	18.84	A
	ATOM	1939	CG	LYS	Α	315	36.280	25.885	34.368	1.00	19.62	A
40	ATOM	1940	CD	LYS			35.653	24.696	35.073		19.22	A
	ATOM	1941	CE	LYS		315	35.070	25.095	36.427		21.00	AC1
	ATOM	1942	NZ	LYS		315	36.119	25.552	37.381		19.53	AC1
	ATOM	1943	C	LYS	n.		38.452	26.393	31.218		18.96	A
	ATOM	1944	Ö	LYS			39.511	25.873	31.561		19.85	A
45	ATOM	1945	N	LEU			38.164	26.691	29.950		17.08	A
43												
	ATOM	1946	CA	LEU			39.102	26.429	28.854		16.41	A
	MOTA	1947	CB	LEU			38.414	25.636	27.738		13.81	A
	MOTA	1948	CG	LEU			38.028	24.201	28.115		14.39	A
	MOTA	1949		LEU			37.139	23.597	27.031		12.38	A
50	MOTA	1950		LEU			39.302	23.373	28.309		12.77	A
	MOTA	1951	C	LEU	Α	316	39.652	27.743	28.290	1.00	17.12	A
	MOTA	1952	0	LEU	Α	316	40.851	27.860	28.023	1.00	16.53	A
	ATOM	1953	N	LEU	Α	317	38.780	28.729	28.105	1.00	16.27	A
	ATOM	1954	CA	LEU		317	39.228	30.022	27.596		17.52	A
55	ATOM	1955	CB	LEU		317	38.083	30.752	26.887		16.37	A
	ATOM	1956	CG	LEU		317	37.448	29.973	25.727		18.81	A
	ATOM	1957		LEU		317	36.415	30.851	25.018		16.47	A
	ATOM	1958		LEU			38.528	29.526	24.741		17.87	A
	ATOM	1959	CDZ	LEU			39.745	30.841	28.774		18.27	A
	AIUN	Tana	-	±E0	м	J 1 /	33.143	20.041	20.114	1.00	10.21	n

	ATOM	1960	0	LEU	Α	317	39.078	31.753	29.273	1.00 18	3.58	Α
	ATOM	1961	N	VAL	Α	318	40.937	30.475	29.229	1.00 18	3.02	A
	ATOM	1962	CA	VAL	Α	318	41.593	31.141	30.342	1.00 18	8.85	A
	ATOM	1963	CB	VAL	Α	318	41.846	30.153	31.500	1.00 19	9.91	A
5	ATOM	1964	CG1	VAL			42.590	30.848	32.634	1.00 20		А
	ATOM	1965		VAL			40.520	29.584	31,990	1.00 19		A
	ATOM	1966	C	VAL			42.923	31.657	29.811	1.00 19		A
	ATOM	1967	ō	VAL			43.690	30.902	29.208	1.00 18		A
	ATOM	1968	N	LEU			43.197	32.939	30.028	1.00 20		A
10	ATOM	1969	CA	LEU			44.436	33.533	29.538	1.00 20		A
	ATOM	1970	CB	LEU			44.521	35.002	29.968	1.00 2		A
	ATOM	1971	CG	LEU			43.418	35.908	29.408	1.00 24		A
	ATOM	1972		LEU			43.606	37.332	29.935	1.00 2		A
	ATOM	1973		LEU			43.453	35.887	27.875	1.00 24		A
15	ATOM	1974	C C	LEU			45.680	32.774	29.994	1.00 20		A
13												
	ATOM	1975	0	LEU			46.568	32.496	29.192	1.00 21		A
	ATOM	1976	N	ASP			45.742	32.440	31.280	1.00 20		A
	MOTA	1977	CA	ASP			46.879	31.707	31.833	1.00 20		A
	ATOM	1978	CB	ASP			46.842	31.760	33.365	1.00 20		A
20	MOTA	1979	CG	ASP			48.049	31.102	34.004	1.00 21		A
	MOTA	1980		ASP			48.669	30.226	33.367	1.00 23		A
	MOTA	1981		ASP			48.371	31.450	35.159	1.00 23		A
	ATOM	1982	С	ASP			46.814	30.247	31.367	1.00 20		A
	MOTA	1983	0	ASP			45.988	29.476	31.840	1.00 20		A
25	ATOM	1984	N	ALA			47.700	29.876	30.451	1.00 20		A
	ATOM	1985	CA	ALA			47.733	28.522	29.903	1.00 22		A
	MOTA	1986	CB	ALA			48.860	28.411	28.881	1.00 20	75	A
	MOTA	1987	C	ALA	Α	321	47.858	27.400	30.940	1.00 21		A
	ATOM	1988	0	ALA	Α	321	47.482	26.259	30.665	1.00 21	L.99	A
30	ATOM	1989	N	THR	Α	322	48.372	27.715	32.127	1.00 20	.89	A
	ATOM	1990	CA	THR	Α	322	48.531	26.698	33.167	1.00 20	0.82	A
	ATOM	1991	CB	THR	Α	322	49.670	27.051	34.146	1.00 19	9.47	A
	ATOM	1992	OG1	THR	Α	322	49.341	28.253	34.848	1.00 20).19	A
	ATOM	1993	CG2	THR	Α	322	50.981	27.249	33.394	1.00 21	L.59	A
35	ATOM	1994	С	THR	Α	322	47.264	26.498	33.983	1.00 19	.55	A.
	ATOM	1995	0	THR			47.235	25.673	34.894	1.00 21		A
	ATOM	1996	N	LYS	А	323	46.216	27.248	33.661	1.00 19	9.33	A
	ATOM	1997	CA	LYS			44.962	27.122	34.392	1.00 21		A
	ATOM	1998	CB	LYS	А	323	44.580	28.460	35.030	1.00 23	3.75	A
40	ATOM	1999	CG	LYS	Α	323	45.562	28.933	36.084	1.00 28	3.45	A
	ATOM	2000	CD	LYS	А	323	45.055	30.177	36.799	1.00 33	3.76	A
	ATOM	2001	CE	LYS	Α	323	46.087	30.678	37.802	1.00 36	5.15	А
	ATOM	2002	NZ	LYS	А	323	46.532	29.569	38.693	1.00 37	7.34	A
	ATOM	2003	С	LYS			43.806	26.614	33.539	1.00 20	.68	A
45	ATOM	2004	0	LYS			42.649	26.757	33.915	1.00 20		А
	ATOM	2005	N	ARG			44.114	26.019	32.392	1.00 19		A
	ATOM	2006	CA	ARG			43.060	25.494	31.531	1.00 17		A
	ATOM	2007	CB	ARG			43.461	25.609	30.061	1.00 15		A
	ATOM	2008	CG	ARG			43.534	27.050	29.603	1.00 17		A
50	ATOM	2009	CD	ARG			43.996	27.194	28.172	1.00 19		A
50	ATOM	2010	NE	ARG			44.438	28.565	27.944	1.00 16		A
	ATOM	2011	CZ	ARG			45.410	28.908	27.108	1.00 19		A
	ATOM	2011		ARG			46.045	27.978	26.398	1.00 1		A
	ATOM	2012		ARG			45.774	30.181	27.015	1.00 1		A
55												
55	ATOM	2014	C	ARG			42.762	24.046	31.883	1.00 18		A
	ATOM	2015	0	ARG			43.673	23.222	32.006	1.00 18		A
	ATOM	2016	N	LEU			41.479	23.748	32.055	1.00 18		A
	MOTA	2017	CA	LEU			41.050	22.403	32.395	1.00 17		A
	MOTA	2018	CB	LEU	Α	325	39.523	22.335	32.425	1.00 17	1.03	A

ATOM 2020 CD1 LBU A 325 39.392 21.048 34.557 1.00 15.93 A ATOM 2021 CD LBU A 325 37.375 21.255 33.084 1.00 16.56 A ATOM 2022 C LBU A 325 41.599 21.433 31.356 1.00 18.08 A ATOM 2024 N GIV A 326 42.354 20.439 31.821 1.00 18.18 A ATOM 2024 N GIV A 326 42.354 20.439 31.821 1.00 18.18 A ATOM 2025 CA GIV A 326 42.931 19.462 30.915 1.00 18.28 A ATOM 2025 CA GIV A 326 42.931 19.462 30.915 1.00 18.28 A ATOM 2026 C GIV A 326 42.931 19.462 30.915 1.00 18.28 A ATOM 2027 O GIV A 326 44.443 19.558 30.807 1.00 19.52 A ATOM 2027 O GIV A 326 45.093 18.592 30.807 1.00 19.52 A ATOM 2028 N CVS A 327 45.016 20.708 31.621 1.00 19.52 A ATOM 2029 CA CVS A 327 46.463 20.867 31.075 1.00 19.30 A ATOM 2028 C CVS A 327 46.866 22.350 31.058 1.00 20.222 A ATOM 2031 CS CVS A 327 46.866 22.350 31.058 1.00 20.222 A ATOM 2031 CS CVS A 327 46.762 23.200 32.649 1.00 21.93 A ATOM 2031 CS CVS A 327 47.169 20.157 32.228 1.00 20.222 A ATOM 2032 C CVS A 327 47.169 20.157 32.228 1.00 20.22 A ATOM 2033 C CVS A 327 47.169 20.157 32.228 1.00 20.22 A ATOM 2035 CA GIU A 328 48.463 19.933 32.263 1.00 20.251 A ATOM 2035 CA GIU A 328 49.274 19.244 33.042 1.00 23.34 A ATOM 2037 CG GIU A 328 50.754 18.507 31.175 1.00 38.24 A ATOM 2039 CD GIU A 328 50.754 18.507 31.175 1.00 38.24 A ATOM 2039 CD GIU A 328 50.754 18.507 31.175 1.00 38.24 A ATOM 2039 CD GIU A 328 50.754 18.507 31.175 1.00 38.24 A ATOM 2039 CD GIU A 328 50.754 18.507 31.175 1.00 38.24 A ATOM 2040 CS GIU A 328 50.754 18.507 31.175 1.00 20.356 A ATOM 2040 CS GIU A 328 50.754 18.507 31.175 1.00 20.271 A ATOM 2040 CS GIU A 328 50.754 18.507 31.175 1.00 20.36 A ATOM 2040 CS GIU A 328 50.754 18.507 31.175 1.00 20.36 A ATOM 2040 CS GIU A 328 50.754 18.507 31.175 1.00 20.376 A ATOM 2040 CS GIU A 328 50.754 18.507 31.175 1.00 20.36 A ATOM 2040 CS GIU A 329 50.13 21.315 1.315 1.00 10.0 20.27 A ATOM 2040 CS GIU A 329 50.50 31.00 20.37 A ATOM 2040 CS GIU A 329 50.50 31.00 20.37 A ATOM 2040 CS GIU A 329 50.50 31.00 20.37 A ATOM 2040 CS GIU A 329 50.20 20.30 31.60 31.60 20.11 A ATOM 2040 CS GIU A 331 46.60 21.21 23		ATOM	2019	CG	LEU	Α	325	38.896	21.125	33.116	1.00	15.91	A
ATOM 2022 C LBU A 325 41,347 21,586 30,157 1,00 18,08 A		ATOM	2020	CD1	LEU	Α	325	39.392	21.048	34.557	1.00	15.93	A
S		ATOM	2021	CD2	LEU	Α	325	37.375	21.255	33.084	1.00	16.56	A
ATOM		ATOM	2022	C	LEU	Α	325	41.599	21.433	31.356	1.00	18.68	A
ATOM 2025 CA GIY A 326 42.931 19.462 30.915 1.00 16.36 A ATOM 2027 C GIY A 326 44.443 19.558 30.807 1.00 19.15 ATOM 2027 C GIY A 326 45.093 18.592 30.404 1.00 19.15 A ATOM 2028 N CYS A 327 45.016 20.708 31.051 1.00 19.30 A ATOM 2029 CA CYS A 327 45.016 20.708 31.055 1.00 19.30 A ATOM 2030 CB CYS A 327 46.463 20.667 31.075 1.00 19.30 A ATOM 2031 CB CYS A 327 46.865 22.350 31.058 1.00 20.22 A ATOM 2031 CB CYS A 327 46.865 22.350 31.058 1.00 20.22 A ATOM 2032 C CYS A 327 46.766 22.350 31.058 1.00 20.22 A ATOM 2033 C CYS A 327 46.561 19.828 33.246 1.00 17.92 A ATOM 2034 C CYS A 327 46.561 19.828 33.246 1.00 17.92 A ATOM 2035 CA GUY A 328 49.274 19.244 31.00 20.51 A ATOM 2035 CA GUY A 328 49.274 19.244 31.00 20.51 A ATOM 2036 CB GUY A 328 50.710 19.139 32.507 1.00 28.68 A ATOM 2037 CG GUY A 328 50.710 19.139 32.507 1.00 28.68 A ATOM 2039 CB GUY A 328 50.710 19.139 32.507 1.00 28.68 A ATOM 2039 CB GUY A 328 52.667 18.500 30.414 1.00 43.23 A ATOM 2040 CB GUY A 328 52.667 18.500 30.414 1.00 43.23 A ATOM 2040 CB GUY A 328 52.657 19.643 30.218 1.00 20.127 A ATOM 2040 CB GUY A 328 49.274 19.161 35.437 1.00 22.11 A ATOM 2040 CB GUY A 328 49.248 19.876 34.455 1.00 22.11 A ATOM 2040 CB GUY A 328 49.248 19.876 34.455 1.00 22.11 A ATOM 2040 CB GUY A 328 49.247 19.161 35.437 1.00 22.17 A ATOM 2044 C GUY A 328 49.248 21.875 35.801 1.00 20.13 A ATOM 2044 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2044 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2044 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2045 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2046 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2046 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2046 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2046 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2046 C GUY A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2046 C GUY A 329 49.248 21.875 33.886 1.00 27.19 A ATOM 2040 C C GUY A 329 49.248 21.875 33.886 1.00 27.19 A ATOM 2040 C C GUY A 329 49.248 21.375 33.886 1.00 27.19 A ATOM 2040 C C GUY A 33	5	ATOM	2023	0	LEU	Α	325	41.347	21.586	30.157	1.00	18.28	A
ATOM 2026 C GLY A 326 44.443 19.558 30.807 1.00 19.55 A ATOM 2028 C GLY A 326 45.093 18.592 30.404 1.00 19.52 A ATOM 2028 C CVS A 327 46.463 20.867 31.161 1.00 18.16 A ATOM 2030 CB CVS A 327 46.463 20.867 31.075 1.00 19.30 ATOM 2030 CB CVS A 327 46.963 20.867 31.055 1.00 20.22 A ATOM 2031 SG CVS A 327 46.965 22.350 31.058 1.00 20.22 A ATOM 2031 SG CVS A 327 46.769 23.200 31.058 1.00 20.22 A ATOM 2032 C CVS A 327 46.769 20.157 32.228 1.00 21.97 A ATOM 2032 C CVS A 327 46.561 19.282 33.200 31.058 1.00 21.97 A ATOM 2033 CB CVS A 327 46.561 19.282 33.200 32.649 1.00 21.97 A ATOM 2034 N GUU A 328 48.463 19.933 32.053 1.00 20.51 A ATOM 2035 CA GUU A 328 49.274 19.244 33.042 1.00 20.51 A ATOM 2035 CA GUU A 328 49.274 19.244 33.042 1.00 20.33 4 A ATOM 2035 CB GUU A 328 50.710 19.139 32.507 1.00 22.58 A ATOM 2037 CG GUU A 328 50.710 19.139 32.507 1.00 28.568 A ATOM 2030 CD GUU A 328 50.710 19.139 32.507 1.00 28.568 A ATOM 2030 CD GUU A 328 52.067 18.507 30.414 1.00 43.23 A ATOM 2040 CB2 GUU A 328 52.067 18.507 30.414 1.00 43.23 A ATOM 2040 CB2 GUU A 328 52.618 17.459 29.991 1.00 44.90 A ATOM 2041 C GUU A 328 49.274 19.244 31.455 1.00 22.11 A ATOM 2041 C GUU A 328 49.247 19.161 35.437 1.00 22.17 A ATOM 2044 CA GUU A 329 49.248 21.875 35.801 1.00 22.11 A ATOM 2045 CB GUU A 329 49.248 21.875 35.801 1.00 22.11 A ATOM 2045 CB GUU A 329 49.248 21.875 35.801 1.00 22.11 A ATOM 2045 CB GUU A 329 49.248 21.875 35.801 1.00 22.13 A ATOM 2045 CB GUU A 329 49.248 21.875 35.801 1.00 22.13 A ATOM 2045 CB GUU A 329 51.014 23.518 33.688 1.00 25.93 A ATOM 2047 CD GUU A 329 49.248 21.875 35.801 1.00 22.97 A ATOM 2048 CB GUU A 329 51.014 23.518 33.188 1.00 27.19 A ATOM 2045 CB GUU A 329 51.014 23.518 33.188 1.00 27.19 A ATOM 2047 CD GUU A 329 49.248 21.875 35.801 1.00 22.95 A ATOM 2049 CB GUU A 329 51.014 23.518 33.188 1.00 27.19 A ATOM 2040 CB GUU A 329 51.014 23.518 33.188 1.00 27.19 A ATOM 2040 CB GUU A 329 51.014 23.518 33.188 1.00 27.19 A ATOM 2040 CB GUU A 329 51.014 23.518 33.188 1.00 27.19 A ATOM 2040 CB GUU A 339 44.745 21.222 36.6		MOTA	2024	N	GLY	Α	326	42.354	20.439	31.821	1.00	18.18	A
ATOM 2027 C		ATOM	2025	CA	GLY	Α	326	42.931	19.462	30.915	1.00	16.36	A
10		MOTA	2026	C	GLY	Α	326	44.443	19.558	30.807	1.00	19.15	A
ATOM 2029 CA CYS A 327 46.863 20.867 31.075 1.00 19.30 A ATOM 2030 CB CYS A 327 46.865 22.350 31.058 1.00 20.22 ATOM 2031 SG CYS A 327 46.786 22.350 31.058 1.00 20.22 ATOM 2032 C CYS A 327 47.169 20.157 32.228 1.00 20.22 ATOM 2032 C CYS A 327 47.169 20.157 32.228 1.00 20.22 A ATOM 2033 C CYS A 327 47.169 20.157 32.228 1.00 20.22 A ATOM 2033 C CYS A 327 47.169 20.157 32.228 1.00 20.22 A ATOM 2034 N GUU A 328 49.274 19.243 32.265 1.00 20.52 A ATOM 2035 CA GUU A 328 49.274 19.243 32.255 1.00 20.51 A ATOM 2036 CB GUU A 328 50.710 19.24 33.245 1.00 20.51 A ATOM 2037 CG GUU A 328 50.710 19.24 33.2507 1.00 28.68 A ATOM 2039 CD GUU A 328 50.710 19.24 33.2507 1.00 28.68 A ATOM 2039 CD GUU A 328 50.710 19.24 18.367 31.75 1.00 44.90 A ATOM 2040 OEZ GUU A 328 52.657 19.500 30.414 1.00 43.23 A ATOM 2041 C GUU A 328 52.658 19.643 30.218 1.00 46.22 A ATOM 2041 C GUU A 328 52.658 19.643 30.218 1.00 46.22 A ATOM 2044 C GUU A 328 49.243 19.876 34.455 1.00 22.11 A ATOM 2044 C GUU A 329 49.276 21.204 34.50 1.00 22.11 A ATOM 2045 CB GUU A 329 49.276 21.204 34.50 1.00 20.13 A ATOM 2046 CG GUU A 329 49.268 21.207 35.667 1.00 20.36 A ATOM 2047 CD GUU A 329 49.268 21.207 35.667 1.00 20.36 A ATOM 2040 CG GUU A 329 51.014 23.561 35.190 1.00 20.35 A ATOM 2040 CG GUU A 329 51.191 23.518 33.688 1.00 20.35 A ATOM 2040 CG GUU A 329 51.191 23.518 33.688 1.00 20.35 A ATOM 2040 CG GUU A 329 51.191 23.518 33.198 1.00 20.36 A ATOM 2040 CG GUU A 329 50.213 23.154 32.995 1.00 26.61 A ATOM 2040 CG GUU A 329 50.213 23.154 32.995 1.00 26.61 A ATOM 2040 CG GUU A 329 50.213 23.154 32.995 1.00 26.61 A ATOM 2050 C GUU A 329 47.775 21.879 37.694 1.00 17.05 A ATOM 2050 C GUU A 329 47.775 21.879 37.694 1.00 17.05 A ATOM 2050 C GUU A 330 44.50 21.20 33.688 1.00 27.19 A ATOM 2050 C GUU A 330 45.527 19.730 36.422 1.00 14.30 A ATOM 2050 C GUU A 331 46.683 21.155 35.691 1.00 20.16 A ATOM 2050 C GUU A 331 46.683 21.155 35.691 1.00 20.16 A ATOM 2050 C GUU A 331 46.683 21.155 33.198 1.00 17.66 A ATOM 2050 C GUU A 331 46.692 1.00 18.00 17.65 A ATOM 2050 C GUU A 331 46		MOTA	2027	0	GLY	Α	326	45.093	18.592	30.404	1.00	19.52	A
ATOM 2030 CB CYS A 327 46.856 22.350 31.058 1.00 20.22 A ATOM 2031 SG CYS A 327 46.762 23.200 32.649 1.00 21.97 ATOM 2032 C CYS A 327 47.169 20.157 32.228 1.00 20.22 A ATOM 2033 C CYS A 327 46.561 19.228 33.20 32.269 1.00 21.97 ATOM 2034 N GUU A 328 46.463 19.933 32.053 1.00 20.51 A ATOM 2035 CA GUU A 328 49.274 19.244 33.042 1.00 20.23 4 ATOM 2035 CA GUU A 328 50.710 19.139 32.507 1.00 22.51 A ATOM 2037 CG GUU A 328 50.710 19.139 32.507 1.00 22.58 A ATOM 2038 CD GUU A 328 50.754 18.367 31.075 1.00 32.34 A ATOM 2039 CD GUU A 328 52.067 18.500 30.414 1.00 43.23 A ATOM 2039 CD GUU A 328 52.067 18.500 30.414 1.00 43.23 A ATOM 2040 082 GUU A 328 52.668 17.459 29.991 1.00 46.22 A ATOM 2040 082 GUU A 328 52.668 17.459 29.991 1.00 46.22 A ATOM 2041 C GUU A 328 52.668 17.459 29.991 1.00 46.22 A ATOM 2041 C GUU A 328 49.234 19.876 44.435 1.00 22.11 A ATOM 2044 CA GUU A 328 49.247 19.161 35.437 1.00 22.17 A ATOM 2044 CA GUU A 329 49.248 21.875 35.801 1.00 22.11 A ATOM 2045 CB GUU A 329 49.248 21.875 35.801 1.00 20.13 A ATOM 2046 CG GUU A 329 49.248 21.875 35.801 1.00 20.36 A ATOM 2047 CD GUU A 329 50.213 23.154 32.995 1.00 25.61 A ATOM 2049 CBU GUU A 329 50.213 23.154 32.995 1.00 25.61 A ATOM 2049 CBU GUU A 329 50.213 23.154 32.995 1.00 25.61 A ATOM 2049 CBU GUU A 329 50.213 23.154 32.995 1.00 25.61 A ATOM 2049 CBU GUU A 329 50.213 23.154 32.995 1.00 25.61 A ATOM 2040 CBU GUU A 329 50.213 23.154 32.995 1.00 25.61 A ATOM 2050 C GUU A 329 50.213 23.154 35.691 1.00 17.28 A ATOM 2050 C GUU A 339 47.789 21.718 36.691 1.00 17.28 A ATOM 2050 C GUU A 339 47.789 21.718 36.691 1.00 17.28 A ATOM 2050 C GUU A 339 47.789 21.718 36.691 1.00 17.28 A ATOM 2050 C GUU A 339 47.789 21.718 36.691 1.00 17.28 A ATOM 2050 C GUU A 339 47.789 21.718 36.691 1.00 17.28 A ATOM 2050 C GUU A 339 47.890 21.718 36.691 1.00 17.28 A ATOM 2050 C GUU A 339 47.789 21.718 36.691 1.00 17.28 A ATOM 2050 C GUU A 331 46.689 17.75 21.894 3.00 10.0 15.39 A ATOM 2050 C GUU A 331 46.689 17.75 21.894 30.0 17.66 A ATOM 2050 C GUU A 331 46.689 17.75 21.894 30.00 17.66	10	MOTA	2028	N	CYS	Α	327	45.016	20.708	31.161	1.00	18.16	A
ATOM 2031 SG CYS A 327 46.782 23.200 32.649 1.00 21.97 A ATOM 2032 C CYS A 327 46.561 19.828 33.246 1.00 20.222 A ATOM 2033 O CYS A 327 46.561 19.828 33.246 1.00 20.22 A ATOM 2034 N GUU A 328 48.463 19.933 32.653 1.00 20.51 A ATOM 2035 CA GUU A 328 49.274 19.244 33.042 1.00 23.34 A ATOM 2036 CB GUU A 328 50.710 19.139 32.507 1.00 28.58 A ATOM 2037 CG GUU A 328 50.754 18.367 31.175 1.00 38.24 A ATOM 2039 CD GUU A 328 50.754 18.367 31.175 1.00 38.24 A ATOM 2039 CD GUU A 328 52.535 19.643 30.218 1.00 44.90 A ATOM 2040 002 GUU A 328 52.535 19.643 30.218 1.00 44.90 A ATOM 2041 C GUU A 328 49.274 19.245 34.455 1.00 22.11 A ATOM 2041 C GUU A 328 49.274 19.459 29.91 1.00 44.90 A ATOM 2041 C GUU A 328 49.247 19.610 35.437 1.00 20.27 A ATOM 2040 CO GUU A 328 49.247 19.610 35.437 1.00 20.21 A ATOM 2040 CO GUU A 329 49.276 21.204 34.506 1.00 22.11 A ATOM 2040 CG GUU A 329 49.276 21.204 34.506 1.00 22.11 A ATOM 2044 CA GUU A 329 49.276 21.204 34.506 1.00 20.13 A ATOM 2045 CB GUU A 329 49.276 21.204 35.657 1.00 20.36 A ATOM 2046 CG GUU A 329 49.575 35.801 1.00 20.13 A ATOM 2047 CD GUU A 329 49.575 35.801 1.00 20.13 A ATOM 2048 CG GUU A 329 51.014 23.518 33.688 1.00 20.35 A ATOM 2049 ORZ GUU A 329 51.014 23.518 33.688 1.00 20.35 A ATOM 2049 ORZ GUU A 329 51.014 23.518 35.195 1.00 26.51 A ATOM 2050 C GUU A 329 51.014 23.518 35.195 1.00 27.19 A ATOM 2050 C GUU A 329 50.213 23.154 32.995 1.00 26.61 A ATOM 2050 C GUU A 329 47.775 21.879 37.694 1.00 17.02 A ATOM 2050 C GUU A 329 47.757 21.879 37.694 1.00 17.05 A ATOM 2050 C GUU A 329 47.757 21.879 37.694 1.00 17.05 A ATOM 2050 C GUU A 330 44.747 21.833 35.294 1.00 17.06 A ATOM 2050 C GUU A 331 45.527 12.793 36.622 1.00 10.0 12.36 A ATOM 2050 C GUU A 331 45.527 12.793 36.622 1.00 10.0 15.30 A ATOM 2050 C GUU A 331 45.527 12.793 36.622 1.00 17.00 16.38 A ATOM 2050 C GUU A 331 46.632 1.115 35.691 1.00 17.06 A ATOM 2050 C GUU A 331 46.507 17.155 37.862 1.00 17.06 A ATOM 2050 C GUU A 331 46.507 17.155 37.862 1.00 17.00 18.67 A ATOM 2060 COZ GUU A 331 46.507 17.155 37.862 1.00 17.46 A A		MOTA	2029	CA	CYS	Α	327	46.463			1.00	19.30	A
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ATOM 2076 CG TYR A 333 43.153 14.683 28.752 1.00 16.46 A													

	ATOM	2078	CE1	TYR	А	333	42.573	16.002	26.794	1.00 13	.42 A	
	ATOM	2079	CD2	TYR			44.490	15.039	28.561	1.00 14		
	ATOM	2080	CE2	TYR			44.872	15.877	27.499	1.00 14		
	ATOM	2081	CZ			333	43.902	16.353	26.626	1.00 15		
5	ATOM	2082	OH			333	44.244	17.197	25.599	1.00 17		
,	ATOM	2083	C			333	41.470	14.230	32.127	1.00 15		
	ATOM	2084	Ö			333	40.278	14.230	31.846	1.00 16		
	ATOM	2085	N			334	41.907	13.650	33.244	1.00 15		
	MOTA	2086	CA			334	40.957	13.100	34.202	1.00 15		
10	ATOM	2087	С			334	39.925	14.146	34.616	1.00 16		
	MOTA	2088	0			334	38.724	13.946	34.433	1.00 15		
	ATOM	2089	N			335	40.366	15.278	35.184	1.00 14		
	MOTA	2090	CD	PRO	Α	335	41.727	15.531	35.689	1.00 15	.88 A	
	MOTA	2091	CA	PRO	Α	335	39.444	16.339	35.606	1.00 15	.29 A	
15	ATOM	2092	CB	PRO	Α	335	40.383	17.397	36.178	1.00 13	.19 A	
	ATOM	2093	CG	PRO	Α	335	41.485	16.569	36.758	1.00 13	.81 A	
	MOTA	2094	C	PRO	Α	335	38.594	16.877	34.448	1.00 15	.84 A	
	ATOM	2095	0	PRO	Α	335	37.423	17.204	34.631	1.00 14	.84 A	
	ATOM	2096	N	LEU	Α	336	39.184	16.971	33.257	1.00 16	.12 A	
20	ATOM	2097	CA	LEU			38.450	17.465	32.094	1.00 15		
	ATOM	2098	CB			336	39.396	17.653	30.898	1.00 14		
	ATOM	2099	CG			336	38.770	17.991	29.538	1.00 15		
	ATOM	2100		LEU			37.836	19.182	29.662	1.00 11		
	ATOM	2101		LEU			39.884	18.285	28.528	1.00 14		
25	ATOM	2102	C			336	37.321	16.508	31.714	1.00 16		
23			Ö						31.540			
	ATOM	2103		LEU			36.176	16.921		1.00 15		
	ATOM	2104	N	LYS			37.640	15.225	31.592	1.00 17		
	MOTA	2105	CA	LYS			36.624	14.243	31.235	1.00 17		
	MOTA	2106	CB			337	37.293	12.900	30.921	1.00 17		
30	MOTA	2107	CG			337	38.170	12.994	29.676	1.00 22		
	MOTA	2108	CD	LYS			39.213	11.892	29.592	1.00 24		
	ATOM	2109	CE			337	38.620	10.560	29.189	1.00 24		
	MOTA	2110	NZ			337	39.710	9.560	28.997	1.00 25		
	MOTA	2111	С	LYS			35.577	14.096	32.342	1.00 17		
35	ATOM	2112	0	LYS	Α	337	34.456	13.652	32.090	1.00 14	.42 A	
	ATOM	2113	N	ALA	Α	338	35.928	14.500	33.559	1.00 15	.83 A	
	ATOM	2114	CA	ALA	Α	338	34.989	14.395	34.674	1.00 17	.52 A	
	MOTA	2115	CB	ALA	A	338	35.749	14.167	35.980	1.00 19	.68 A	
	ATOM	2116	C	ALA	Α	338	34.095	15.621	34.804	1.00 18	.83 A	
40	ATOM	2117	0	ALA	Α	338	33.252	15.687	35.695	1.00 18	.94 A	
	ATOM	2118	N	HIS			34.262	16.596	33.918	1.00 19		
	ATOM	2119	CA	HIS			33.438	17.796	34.004	1.00 19		
	ATOM	2120	CB	HIS			33.865	18.819	32.949	1.00 19		
	ATOM	2121	CG	HIS			33.163	20.134	33.074	1.00 20		
45	ATOM	2122		HIS			33.549	21.299	33.649	1.00 18		
75	ATOM	2123		HIS			31.880	20.340	32.612	1.00 19		
	ATOM	2124		HIS			31.506	21.576	32.896	1.00 22		
	ATOM	2125		HIS			32.500	22.179	33.525	1.00 21		
50	ATOM	2126	C	HIS			31.957	17.448	33.845	1.00 19		
50	ATOM	2127	0	HIS			31.597	16.576	33.061	1.00 19		
	MOTA	2128	N			340	31.079	18.125	34.606	1.00 19		
	MOTA	2129	CD			340	31.424	19.119	35.640	1.00 19		
	MOTA	2130	CA			340	29.630	17.900	34.569	1.00 20		
	ATOM	2131	CB			340	29.091	19.058	35.396	1.00 20		
55	MOTA	2132	CG			340	30.146	19.207	36.454	1.00 19		
	MOTA	2133	C			340	29.000	17.834	33.176	1.00 21		
	MOTA	2134	0	PRO	Α	340	28.049	17.088	32.955	1.00 22	.48 A	
	ATOM	2135	N	PHE	Α	341	29.528	18.606	32.237	1.00 21	.33 A	
	ATOM	2136	CA	PHE	Α	341	28.985	18.610	30.886	1.00 21	.57 A	

	ATOM	2137	CB	PHE	A	341	29.739	19.624	30.017	1.00	21.64	A
	ATOM	2138	CG	PHE			29.207	19.740	28.613		23.18	A
	ATOM	2139		PHE			27.903	20.171	28.382		22.58	A
	ATOM	2140	CD2			341	30.013	19.431	27.522		21.95	A
5	ATOM	2141	CE1	PHE			27.410	20.292	27.082		23.54	A
,	ATOM	2142	CE2	PHE			29.533	19.548	26.220		21.83	A
		2142	CZ	PHE				19.980			23.23	A
	ATOM						28.228		25.998			
	MOTA	2144	C	PHE			29.055	17.226	30.237		21.84	A
10	MOTA	2145	0	PHE			28.232	16.896	29.389		20.37	A
10	MOTA	2146	N	PHE			30.034	16.422	30.640		20.51	A
	MOTA	2147	CA	PHE			30.221	15.085	30.077		23.01	A
	ATOM	2148	CB	PHE			31.710	14.809	29.850		18.00	A
	MOTA	2149	CG	PHE			32.398	15.812	28.971		17.05	A
	ATOM	2150		PHE			32.010	15.987	27.652		17.78	A
15	MOTA	2151		PHE			33.487	16.534	29.450		15.72	A
	ATOM	2152	CE1	PHE	Α	342	32.702	16.867	26.811	1.00	18.08	A
	MOTA	2153	CE2	PHE	Α	342	34.184	17.414	28.617	1.00	17.45	A
	MOTA	2154	CZ	PHE	Α	342	33.790	17.578	27.298	1.00	16.56	A
	MOTA	2155	С	PHE	Α	342	29.679	13.972	30.976	1.00	24.95	A
20	ATOM	2156	0	PHE	Α	342	30.002	12.798	30.777	1.00	23.95	A
	ATOM	2157	N	GLU .	Α	343	28.861	14.333	31.958	1.00	27.35	A
	ATOM	2158	CA	GLU	Α	343	28.325	13.349	32.897	1.00	30.28	A
	ATOM	2159	CB	GLU	Α	343	27.187	13.964	33.716	1.00	32.20	A
	ATOM	2160	CG	GLU	A	343	26.581	12.991	34.714	1.00	39.71	A
25	ATOM	2161	CD	GLU			25.628	13.661	35.688		44.72	A
	ATOM	2162		GLU			24.661	14.314	35.234		47.55	A
	ATOM	2163		GLU			25.847	13.526	36.911		46.89	A
	ATOM	2164	C	GLU			27.852	12.017	32.305		28.98	A
	ATOM	2165	ō	GLU			28.225	10.952	32.800		31.73	A
30	ATOM	2166	N	SER			27.037	12.067	31.258		26.09	A
50	ATOM	2167	CA	SER			26.520	10.838	30.656		28.36	A
	ATOM	2168	CB	SER			25.129	11.089	30.067		28.73	A
	ATOM	2169	OG	SER			25.203	11.942	28.940		30.91	A
	ATOM	2170	C	SER			27.407	10.214	29.577		27.66	A
35	ATOM	2171	0	SER			26.987	9.281	28.900		28.66	A
33	ATOM	2172	N	VAL			28.627	10.715	29.419		26.75	A
	ATOM	2173	CA	VAL			29.534	10.713	28.402		23.44	A
		2174	CB	VAL			30.565	11.256	27.950		23.44	A
	ATOM											A
40	ATOM	2175 2176		VAL .			31.589	10.631	26.995		22.24	A
40	ATOM			VAL .			29.854	12.418	27.275		20.05	
	MOTA	2177	C	VAL .			30.326	8.957	28.855		24.26	A
	MOTA	2178	0	VAL			30.876	8.930	29.960		22.83	A
	ATOM	2179	N	THR			30.374	7.942	27.997		21.77	A
	MOTA	2180	CA	THR			31.153	6.740	28.272		23.70	A
45	MOTA	2181	CB	THR			30.391	5.455	27.857		26.53	A
	MOTA	2182		THR			29.248	5.284	28.706		29.98	A
	MOTA	2183		THR			31.289	4.231	27.990		24.28	A
	MOTA	2184	C	THR			32.383	6.945	27.385		23.43	A
	MOTA	2185	0	THR			32.306	6.827	26.160		24.50	A
50	MOTA	2186	N	TRP			33.508	7.270	28.013		22.98	A
	MOTA	2187	CA	TRP	Α	347	34.744	7.569	27.300	1.00	23.81	A
	ATOM	2188	CB	TRP.	Α	347	35.683	8.352	28.219	1.00	22.54	A
	ATOM	2189	CG	TRP	Α	347	35.128	9.658	28.693	1.00	20.61	A
	ATOM	2190	CD2	TRP	Α	347	35.257	10.927	28.040	1.00	19.11	A
55	ATOM	2191	CE2	TRP	Α	347	34.581	11.881	28.838	1.00	18.39	A
	MOTA	2192	CE3	TRP	Α	347	35.878	11.351	26.858	1.00	18.16	A
	MOTA	2193		TRP			34.397	9.883	29.828		18.35	A
	ATOM	2194		TRP			34.065	11.218	29.923		19.51	A
	MOTA	2195		TRP			34.510	13.234	28.491		16.88	A

	ATOM	2196	CZ3	TRP	Α	347	35.808	12.701	26.511	1.00 17.23	A
	ATOM	2197	CH2	TRP	А	347	35.127	13.624	27,327	1.00 18.16	A
	ATOM	2198	C	TRP			35.538	6.429	26.675	1.00 25.79	A
	ATOM	2199	ō	TRP		347	36.304	6.654	25.742	1.00 24.67	A
5	ATOM	2200	N	ALA			35.360	5.215	27.183	1.00 27.10	A
-	ATOM	2201	CA	ALA			36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	CB	ALA			35.899	2.869	27.636	1.00 27.09	A
	ATOM	2202	C	ALA			35.895	3.620	25.256	1.00 27.03	A
	ATOM	2203	0	ALA			36.830	3.148	24.613	1.00 27.18	A
10											
10	ATOM	2205	N	ASN			34.682	3.769	24.735	1.00 26.55	A
	ATOM	2206	CA	ASN			34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	CB	ASN			33.700	1.962	23.444	1.00 29.37	A
	MOTA	2208	CG	ASN			32.299	2.088	24.013	1.00 30.92	A
	ATOM	2209		ASN			32.045	2.942	24.859	1.00 30.17	A
15	MOTA	2210		ASN			31.386	1.237	23.553	1.00 33.52	A
	MOTA	2211	C	ASN			33.599	4.265	22.509	1.00 26.47	A
	MOTA	2212	0	ASN.			32.669	3.843	21.819	1.00 25.87	A
	MOTA	2213	N	LEU .			33.947	5.543	22.518	1.00 24.45	A
	MOTA	2214	CA	LEU .			33.203	6.510	21.721	1.00 23.14	A
20	MOTA	2215	CB	LEU	Α	350	33.837	7.898	21.848	1.00 23.22	A
	MOTA	2216	CG	LEU	Α	350	33.659	8.605	23.191	1.00 21.05	A
	ATOM	2217	CD1	LEU	Α	350	34.646	9.756	23.293	1.00 19.36	A
	ATOM	2218	CD2	LEU	Α	350	32.220	9.094	23.319	1.00 18.78	A
	MOTA	2219	С	LEU	Α	350	33.082	6.152	20.240	1.00 22.60	A
25	ATOM	2220	0	LEU	Α	350	32.011	6.296	19.650	1.00 21.15	A
	ATOM	2221	N	HIS	Α	351	34.165	5.689	19.627	1.00 23.13	A
	ATOM	2222	CA	HIS			34.089	5.387	18.204	1.00 27.83	A
	ATOM	2223	CB	HIS			35.506	5.325	17.596	1.00 29.36	A
	ATOM	2224	CG	HIS			36.082	3.950	17.493	1.00 32.07	A
30	ATOM	2225		HIS			36.611	3.128	18.431	1.00 32.39	A
50	ATOM	2226		HIS			36.197	3.285	16.291	1.00 33.02	A
	ATOM	2227		HIS			36.775	2.113	16.493	1.00 33.58	A
	ATOM	2228		HIS			37.036	1.992	17.782	1.00 33.30	A
	ATOM	2229	C	HIS			33.258	4.144	17.874	1.00 28.12	A
35	ATOM	2230	0	HIS			33.238	3.847	16.707	1.00 29.49	A
33	ATOM	2230	N	GLN			32.800	3.442	18.908	1.00 29.28	A
	ATOM	2231	CA	GLN			31.963	2.255	18.726	1.00 29.28	A
					A						
	ATOM	2233	CB	GLN		352	32.366	1.145	19.694	0.50 30.56	AC1
40	ATOM	2234	CG	GLN		352	33.169	0.041	19.041	0.50 30.88	AC1
40	ATOM	2235	CD	GLN		352	34.493	-0.186	19.729	0.50 31.21	AC1
	ATOM	2236		GLN		352	34.541	-0.450	20.928	0.50 30.76	AC1
	MOTA	2237		GLN		352	35.578	-0.084	18.971	0.50 32.30	AC1
	MOTA	2238	С	GLN			30.504	2.638	18.963	1.00 30.42	A
	MOTA	2239	0	GLN			29.595	1.831	18.770	1.00 29.01	A
45	MOTA	2240	N	GLN			30.290	3.875	19.397	1.00 27.64	A
	MOTA	2241	CA	GLN			28.948	4.365	19.652	1.00 27.42	A
	MOTA	2242	CB	GLN			28.977	5.401	20.775	1.00 25.77	A.
	MOTA	2243	CG	GLN			29.408	4.837	22.115	1.00 27.34	A.
	MOTA	2244	CD	GLN .	A	353	29.638	5.914	23.156	1.00 27.19	A
50	MOTA	2245	OE1	GLN	À	353	28.875	6.872	23.252	1.00 28.29	A
	MOTA	2246	NE2	GLN	Α	353	30.687	5.753	23.951	1.00 28.79	A
	ATOM	2247	C	GLN	Α	353	28.375	4.989	18.385	1.00 29.00	A
	MOTA	2248	0	GLN	Α	353	29.118	5.455	17.516	1.00 29.14	A
	ATOM	2249	N	THR			27.053	4.984	18.276	1.00 27.31	A
55	ATOM	2250	CA	THR			26.390	5.568	17.119	1.00 27.85	A
	ATOM	2251	CB	THR			24.991	4.941	16.904	1.00 30.69	A
	ATOM	2252	OG1				25.132	3.532	16.665	1.00 30.07	A
	ATOM	2253		THR			24.289	5.585	15.709	1.00 29.58	A
	ATOM	2254	C	THR			26.244	7.062	17.376	1.00 26.85	A

	MOTA	2255	0	THR	Α	354	25.592	7.475	18.329	1.00	25.77	A
	ATOM	2256	N	PRO	Α	355	26.867	7.898	16.533	1.00	27.22	A
	ATOM	2257	CD	PRO	Α	355	27.792	7.588	15.431	1.00	25.89	A
	ATOM	2258	CA	PRO		355	26.763	9.346	16.734		27.23	A
5	ATOM	2259	CB	PRO	А	355	27.625	9.915	15.609		24.91	A
	ATOM	2260	CG			355	28.643	8.838	15.385		25.54	A
	ATOM	2261	C			355	25.322	9.837	16.641		28.07	A
	ATOM	2262	ō			355	24.548	9.364	15.810		27.24	A
	ATOM	2263	N			356	24.941	10.792	17.500		28.28	A
10	ATOM	2264	CD			356	25.752	11.560	18.462		28.31	A
	ATOM	2265	CA			356	23.572	11.306	17.448		28.44	A
	ATOM	2266	CB			356	23.539	12.301	18.604		28.11	A
	ATOM	2267	CG			356	24.946	12.832	18.612		26.86	A
	ATOM	2268	c			356	23.363	11.978	16.097		29.25	A
15	ATOM	2269	ō			356	24.304	12.537	15.529		27.27	A
	ATOM	2270	N	ALA			22.143	11.910	15.575		30.45	A
	ATOM	2271	CA	ALA			21.848	12.521	14.287		32.81	A
	ATOM	2272	CB	ALA			20.507	12.019	13.757		31.99	A
	ATOM	2273	C	ALA			21.824	14.035	14.448		35.05	A
20	ATOM	2274	0	ALA			21.194	14.561	15.369		35.04	A
20	ATOM	2275	N			358	22.516	14.730	13.552		37.81	A
	ATOM	2276	CA	LEU			22.578	16.185	13.597		42.15	A
	ATOM	2277	CB	LEU			23.679	16.681	12.658		39.54	A
	ATOM	2278	CG			358	25.086	16.285	13.109		39.51	A A
25	ATOM	2279		LEU			26.102	16.686	12.062		39.29	A A
23	ATOM	2280		LEU			25.395	16.953	14.445		40.01	A
	ATOM	2281	C			358	21.241	16.837	13.242		45.91	A
	ATOM	2282	o	LEU			20.874	16.927	12.069		45.71	A
	ATOM	2283	N			359	20.530	17.290	14.275		50.06	A
30	ATOM	2284	CA			359	19.223	17.230	14.140		53.73	A A
30	ATOM	2285	CB	THR			19.353	19.428	13.726		54.04	A A
	ATOM	2286		THR			19.995	19.521	12.448		56.35	A
	ATOM	2287		THR			20.158	20.204	14.763		54.32	A
	ATOM	2288	C			359	18.309	17.236	13.139		54.47	A
35	ATOM	2289	ō			359	18.483	16.016	12.930		55.90	A
33	ATOM	2290		THR			17.407	17.908	12.595		56.97	A
	ATOM	2291		TIP		1	42.566	19.118	34.302		15.09	S
	ATOM	2292		TIP	S	2	41.052	32.378	19.857		15.82	S
	ATOM	2293		TIP	S	3	37.014	33.030	17.747		16.95	S
40	ATOM	2294		TIP	S	5	45.353	24.370	18.152		16.85	S
40	ATOM	2295		TIP	s	6	31.896	13.930	33.235		20.42	S
	ATOM	2296		TIP	S	7	50.351	22.781	28.249		21.14	S
	ATOM	2297		TIP	S	8	45.246	-0.589	-0.734		17.74	S
	ATOM	2298		TIP	S	11	46.249	-0.348	-8.523		21.32	S
45	ATOM	2299		TIP	S	14	45.756	11.148	29.680		21.94	S
75	ATOM	2300	OH2		S	15	44.273	13.157	34.592		15.61	S
	ATOM	2301		TIP	S	17	53.598	3.722	-1.720		21.45	S
	ATOM	2301		TIP	S	18	46.049	13.087	31.565		20.35	S
	ATOM	2302		TIP	S	19	53.422	22.401	-3.280		23.26	S
50	ATOM	2304		TIP	S	20	34.587	7.922	5.383		22.58	S
50	ATOM	2305		TIP	S	21	45.053	27.379	19.376		29.60	S
	ATOM	2306	OH2			23	28.899	36.416	28.633		31.68	S
	ATOM	2307		TIP	S	24	35.531	11.645	-8.219		23.45	S
	ATOM	2308		TIP	S	25	47.364	28.787	19.612		23.43	S
55	ATOM	2309		TIP	S	27	48.859	21.588	12.634		23.76	S
22	ATOM	2310	OH2		S	29	48.805	8.920	23.626		22.23	S
	ATOM	2311	OH2	TIP	S	31	48.619	7.247	10.112		21.32	S
	ATOM	2311		TIP		34	44.824	28.720	15.621		25.27	S
	ATOM	2312		TIP		35	26.030	12.634	13.407		21.61	S

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	MOTA	2314		TIP		36	50.462	19.810	40.066		25.45	S
	MOTA	2315	OH2	TIP	s	37	39.631	23.510	-0.239		30.88	S
	MOTA	2316	OH2	TIP	S	40	44.734	42.655	10.346	1.00	30.84	S
	MOTA	2317	OH2	TIP	S	41	54.653	3.902	1.503	1.00	27.14	S
5	MOTA	2318	OH2	TIP	s	45	45.693	21.923	39.754	1.00	28.30	S
	MOTA	2319	OH2	TIP	s	47	47,820	16.413	7.805		25.73	S
	ATOM	2320	OH2		S	48	50.292	31.412	29.642		32.79	S
	ATOM	2321	OH2		S	49	26.056	16.646	34.827		29.80	s
	MOTA	2322	OH2	TIP	S	52	31.714	10.996	31.855		29.15	S
10	MOTA	2323	OH2		S	53	46.108	23.843	-4.299		24.21	S
	MOTA	2324	OH2		S	54	37.645	11.206	34.448		28.56	S
	ATOM	2325	OH2	TIP	S	55	26.371	28.513	12.142	1.00	32.08	S
	ATOM	2326	OH2	TIP	s	58	33.564	19.700	3.483	1.00	28.28	S
	ATOM	2327	OH2	TIP	s	64	48.295	-0.632	14.280	1.00	32.13	S
15	MOTA	2328	OH2	TIP	s	65	40.064	26.036	34.324	1.00	24.17	S
	ATOM	2329	OH2	TIP	s	66	29.570	3.958	14.729		28.94	S
	ATOM	2330	OH2	TIP	s	72	60.085	11.604	6.814		38.35	s
	ATOM	2331	OH2	TIP	S	73	39.203	44.403	18.686		26.61	s
												S
20	MOTA	2332	OH2	TIP	S	76	47.312	12.366	27.366		28.51	
20	MOTA	2333	OH2	TIP	s	80	43.862	33.771	33.329		28.82	S
	MOTA	2334	OH2	TIP	S	81	57.890	13.106	2.128		40.62	S
	MOTA	2335	OH2	TIP	S	82	41.663	34.381	32.043		19.35	S
	MOTA	2336	OH2	TIP	s	85	50.974	40.331	19.200	1.00	21.14	S
	ATOM	2337	OH2	TIP	s	88	47.925	-0.832	-6.556	1.00	24.11	S
25	ATOM	2338	OH2	TIP	s	90	27.231	28.336	33.481	1.00	27.64	S
	ATOM	2339	OH2	TIP	s	91	43.651	-7.101	-7.995	1.00	24.33	S
	ATOM	2340	OH2		S	92	49.325	4.387	19.370		28.02	S
	ATOM	2341	OH2	TIP	S	93	46.231	11.549	33.898		29.40	S
	ATOM	2342	OH2	TIP	s	94	63.889	24.831	1.168		26.53	s
30	ATOM	2343	OH2	TIP	s	96	56.396	4.952	-6.749		28.00	s
30												
	MOTA	2344	OH2	TIP	S	98	35.510	27.986	11.558		29.24	S
	MOTA	2345	OH2	TIP	S	100	49.942	24.366	30.265		31.61	S
	MOTA	2346	OH2		S	101	56.121	7.113	-8.298		31.57	S
	MOTA	2347	OH2		S	102	58.318	19.957	-8.378		26.95	S
35	MOTA	2348	OH2	TIP	s	103	49.647	22.446	39.624	1.00	40.57	S
	ATOM	2349	OH2	TIP	S	104	45.359	7.052	13.052	1.00	26.27	S
	MOTA	2350	OH2	TIP	S	105	37.150	32.340	32.346	1.00	34.45	S
	MOTA	2351	OH2	TIP	S	107	43.465	40.457	8.240	1.00	40.48	S
	ATOM	2352	OH2	TIP	s	119	36.644	8.257	13.418	1.00	30.70	S
40	ATOM	2353	OH2	TIP	s	123	41.912	-8.974	-8.264	1.00	26.08	s
	ATOM	2354	OH2			124	62.424	15.800	-7.411		24.08	s
	ATOM	2355	OH2		S	126	37.266	18.656	-9.097		28.99	s
	ATOM	2356		TIP		127	43.129	26.845	14.606		25.19	s
		2357				128			29.802		29.25	S
4.5	MOTA		OH2		S		36.339	32.639				
45	MOTA	2358	OH2			130	54.051	14.561	26.498		33.93	S
	MOTA	2359	OH2	TIP	S	131	41.805	-4.242	5.492		33.72	S
	MOTA	2360		TIP		133	38.873	25.163	36.697		30.69	S
	MOTA	2361	OH2	TIP	S	134	28.777	8.553	25.307	1.00	31.43	S
	ATOM	2362	OH2	TIP	S	135	53.672	10.546	-12.803	1.00	33.45	S
50	MOTA	2363	OH2	TIP	s	136	59.892	15.434	11.467	1.00	31.39	S
	ATOM	2364	OH2	TIP	s	137	31.040	12.361	35.470	1.00	34.07	S
	ATOM	2365	OH2		S	139	33.489	14.292	-0.598		40.68	s
	ATOM	2366		TIP		140	46.918	8.748	11.662		29.23	S
	ATOM	2367	OH2		S	141	46.297	-7.287	-9.196		42.20	S
55	ATOM	2368				141	58.193	6.715	-4.685		35.48	S
23												
	MOTA	2369	OH2	TIP	S	143	44.598	4.435	12.503		27.68	S
	MOTA	2370	OH2	TIP		144	27.003	5.999	12.450		36.30	S
	MOTA	2371	OH2			145	43.676	32.852	35.735		35.70	S
	ATOM	2372	OH2	TIP	S	146	35.783	18.628	36.452	1.00	34.62	S

	ATOM	2373	OH2	TIP	s	147	25.402	4.058	20.638	1.00	45.03	S
	ATOM	2374	OH2	TIP	s	148	45.839	35.853	33.724	1.00	35.47	S
	ATOM	2375	OH2	TIP	S	149	22.176	18.976	16.752		31.87	S
	ATOM	2376				150	43.986	33.179	10.162		37.70	S
5	ATOM	2377				151	50.653	20.347	42.428		35.80	S
-	MOTA	2378		TIP		152	47.843	24.314	9.506		31.05	S
	ATOM	2379	OH2	TIP		153	44.693		-14.175		29.90	S
	ATOM	2380		TIP		155	26.560	36.851	31.684		49.29	S
	ATOM	2381	OH2			156	46.867		-12.951		29.21	S
10				TIP		157	30.432	28.741	12.438		37.76	
10	MOTA	2382										S
	ATOM	2383	OH2	TIP	S	158	41.004	20.553	6.423		39.53	S
	ATOM	2384	OH2			159	49.258	20.069	29.294		33.97	S
	MOTA	2385		TIP		160	48.082	28.459	16.489		33.10	S
	ATOM	2386		TIP		161	47.448	18.625	27.683		34.87	S
15	MOTA	2387	OH2	TIP	s	162	19.687	20.632	23.411		35.01	S
	MOTA	2388	OH2	TIP		163	32.402	-1.266	22.443		37.26	S
	MOTA	2389	OH2	TIP	S	164	39.475	33.468	33.237	1.00	35.34	S
	MOTA	2390	OH2	TIP	S	165	44.277	18.950	5.162		45.14	S
	ATOM	2391	OH2	TIP	s	166	34.797	30.523	10.736	1.00	47.55	S
20	ATOM	2392	OH2	TIP	s	167	46.541	3.526	-14.949	1.00	26.54	S
	MOTA	2393	OH2	TIP	s	168	36.333	16.371	1.539	1.00	38.68	S
	ATOM	2394	OH2	TIP	S	169	46.761	38.936	27.403	1.00	34.66	S
	ATOM	2395	OH2	TIP	s	170	24.163	13.264	11.375	1.00	41.23	S
	ATOM	2396	OH2		s	171	48.459	15.018	31.951		38.11	S
25	ATOM	2397	OH2		S	172	34.261	23.193	40.004		48.96	S
	ATOM	2398	OH2	TIP	s	173	45.924	-0.026	13.224		39.55	S
	ATOM	2399		TIP		175	41.384	37.389	32.543		40.74	S
	ATOM	2400				177	49.394	35.312	27.150		44.33	s
	ATOM	2401		TIP		178	29.066	29.942	34.359		41.46	s
30	ATOM	2402	OH2	TIP	S	180	49.354	19.467	7.273		34.56	S
50	ATOM	2403	OH2			181	25.298	17.029	31.863		47.74	S
	ATOM	2403		TIP		182	37.071	25.027	4.669		43.87	S
	ATOM	2404		TIP		183	22.581	7.487	18.691		41.75	S
2.5	ATOM	2406			S	184	32.269	7.011	-1.891		48.84	S
35	ATOM	2407	OH2	TIP		185	48.234	0.494	6.833		48.16	S
	ATOM	2408	OH2	TIP		187	20.008	14.658	19.211		45.27	S
	ATOM	2409		TIP		188	49.341	22.698	42.272		42.20	S
	MOTA	2410	OH2	TIP		190	61.292	18.260	-8.097		45.21	S
	MOTA	2411		TIP			28.152	10.606	2.819		40.38	S
40	MOTA	2412		TIP		192	25.626	12.619	23.191		34.27	S
	MOTA	2413		TIP		193	59.876	11.603	1.216		46.54	S
	ATOM	2414	OH2			194	57.592	21.183			45.82	S
	ATOM	2415		TIP	S	195	31.509	36.649	21.499		38.73	S
	ATOM	2416	OH2	TIP	S	197	50.270	-1.543	-6.136	1.00	42.66	S
45	MOTA	2417	OH2	TIP	S	198	24.467	8.729	13.088	1.00	42.78	S
	ATOM	2418	OH2	TIP	S	199	38.098	8.699	25.759	1.00	32.80	S
	ATOM	2419	OH2	TIP	S	200	57.831	11.358	-13.255	1.00	45.31	S
	ATOM	2420	OH2	TIP	S	201	23.888	22.328	30.524	1.00	37.12	S
	ATOM	2421	OH2	TIP	S	202	47.691	26.068	37.666	1.00	37.92	S
50	ATOM	2422	OH2	TIP	s	203	38.653	7.070	29.307	1.00	50.54	S
	ATOM	2423	OH2	TIP	S	206	44.424	27.583	2.092	1.00	53.50	S
	ATOM	2424	OH2	TIP		212	22.258	2.296	17.948		47.38	S
	ATOM	2425	OH2	TIP		214	19.843	17.943	23.303		30.36	S
	ATOM	2426		TIP		216	27.647	11.344	24.681		31.32	S
55	ATOM	2427		TIP	S	217	37.953	7.817	-9.284		45.97	S
22	ATOM	2428	OH2			218	33.845	34.040	12.124		38.11	S
	ATOM	2429	OH2	TIP	S	219	58.484	15.269	13.717		38.26	S
	ATOM	2430		TIP			48.526	40.920	26.583		35.23	S
	ATOM	2430		TIP		222	52.094	21.184	38.122		29.86	S
	MIUN	242I	UnZ	TIP	0	444	JZ. U94	41.104	30.122	1.00	47.00	5

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	ATOM	2432	OH2	TIP			36.889		881	3.281		37.63	S
	MOTA	2433	OH2	TIP	S	224	47.642	-1.	401	-10.684	1.00	34.89	S
	ATOM	2434	OH2	TIP	S	226	47.284	2.	916	19.133	1.00	34.10	S
	ATOM	2435	OH2	TIP	S	227	42.468	4.	463	-15.039	1.00	37.98	S
5	ATOM	2436	OH2		s	228	19.169		832	21.831		41.57	S
	ATOM	2437	OH2		s	231	57.592		689	14.880		50.22	s
	ATOM	2438	OH2	TIP		232	27.102		176	5.655		40.57	S
									072				
	MOTA	2439	OH2			233	58.618			-11.925		50.71	S
	MOTA	2440	OH2			234	22.822		342	19.945		34.93	S
10	MOTA	2441	OH2	TIP		236	24.831		218	28.901		37.69	S
	MOTA	2442	OH2	TIP	S	237	20.045	10.	774	16.992		39.57	S
	ATOM	2443	OH2	TIP	S	238	58.019	19.	850	15.679	1.00	41.42	S
	ATOM	2444	OH2	TIP	s	239	19.490	20.	949	26.114	1.00	34.55	S
	ATOM	2445	OH2	TIP	s	240	61.187	26.	377	7.346	1.00	39.68	S
15	ATOM	2446	OH2	TIP	S	241	33.680		342	19.389	1.00	48.93	S
	ATOM	2447	OH2	TIP	s	242	51.539		612	10.881		55.65	s
	ATOM	2448	OH2	TIP		244	25.872		431	30.404		46.69	S
	ATOM	2449	OH2	TIP		248	37.332		849	9.544		43.81	s
													S
20	ATOM	2450	OH2	TIP		250	39.087		293	-9.655		42.96	
20	MOTA	2451	OH2	TIP	S	258	23.938		000	30.010		38.89	S
	MOTA	2452	OH2			259	24.949		749	32.578		40.17	S
	ATOM	2453	OH2		S	260	32.111		986	1.918		48.36	S
	ATOM	2454	OH2	TIP	s	266	21.404	12.	876	25.603	1.00	57.17	S
	ATOM	2455	OH2	TIP	s	269	35.425	36.	767	12.550	1.00	30.70	S
25	ATOM	2456	OH2	TIP	s	270	52.438	25.	529	30.131	1.00	44.85	S
	ATOM	2457	OH2	TIP	s	271	53.299	20.	156	36.003	1.00	37.15	S
	ATOM	2458	OH2	TIP	s	272	50.914	6.	919	23.723	1.00	43.29	s
	ATOM	2459	OH2	TIP	S	274	31.578		795	11.014		50.15	S
	ATOM	2460	OH2		s	275	26.341		243	22.447		39.40	s
30	ATOM	2461	OH2		s	276	60.392		195	10.235		37.91	s
30							47.355			-10.821			
	ATOM	2462	OH2	TIP	S	277						48.18	S
	MOTA	2463	OH2	TIP	S	279	41.304			-16.647		38.12	S
	MOTA	2464	OH2		S	282	33.299		620	37.881		46.29	S
	ATOM	2465	OH2		S	283	56.469		112	-8.575		43.71	S
35	ATOM	2466	OH2	TIP	s	287	48.382	26.	573	7.246	1.00	41.43	S
	ATOM	2467	OH2	TIP	S	288	56.240	7.	245	-11.331	1.00	41.79	S
	MOTA	2468	OH2	TIP	S	290	49.060	14.	978	28.166	1.00	37.03	S
	ATOM	2469	OH2	TIP	S	291	37.095	44.	270	26.442	1.00	45.08	S
	ATOM	2470	OH2	TIP	S	292	47.814	-0.	384	-13.299	1.00	48.60	S
40	ATOM	2471	OH2	TIP	s	297	58.081	2.	784	-7.841	1.00	41.89	S
	ATOM	2472	OH2	TIP	s	298	36.447	45.	321	18.644	1.00	54.91	S
	ATOM	2473	OH2		S	299	49.029		328	1.767		30.55	s
	ATOM	2474	OH2			301	24.375		771	8.634		48.47	s
	ATOM	2475	OH2		S	303	47.904		798	28.653		35.76	s
45		2476	OH2		S	305	51.156		821	27.172		43.59	S
43	ATOM												
	MOTA	2477	OH2	TIP	S	306	32.943		917	35.227		42.60	S
	MOTA	2478		TIP		307	58.462		373	6.251		46.15	S
	MOTA	2479		TIP		308	41.964		940	36.712		48.26	S
	MOTA	2480	OH2				51.176	-1.	922	-3.336	1.00	50.61	S
50	MOTA	2481	OH2	TIP	Sí	1001	21.319	36.	868	23.805	1.00	36.97	S
	MOTA	2482	OH2	TIP	S.	1002	48.880	32.	620	27.617	1.00	44.40	S
	ATOM	2483	OH2	TIP	S.	1003	61.880	19.	473	11.767	1.00	45.49	S
	ATOM	2484	OH2	TIP	S	1004	52.770	21.	424	26.815	1.00	24.43	S
	ATOM	2485	OH2				35.373		094	36.197		35.97	S
55	ATOM	2486		TIP			40.815		636	4.389		43.15	S
22	ATOM	2487	OH2	TIP			44.953		286	11.272		49.45	S
	ATOM	2488	OH2	TIP			21.004		168	27.009		48.51	S
													5 S
	ATOM	2489	OH2				47.094		786	9.243		50.10	
	MOTA	2490	OH2	TIP	S.	1012	32.479	2.	978	14.158	1.00	49.47	S

ATOM	.00 40.72 .00 38.09 .00 38.09 .00 38.09 .00 37.32 .00 36.74 .00 33.52 .00 31.05 .00 31.05 .00 30.70 .00 30.70 .00 30.91	
ATOM	.00 38.05 .00 38.09 .00 33.99 .00 33.39 .00 36.74 .00 36.74 .00 31.05 .00 31.05 .00 31.05 .00 30.70 .00 30.70 .00 30.70 .00 30.03 .00 39.52 .00 39.52 .00 39.52 .00 30.03 .00 30.03	
ATOM	.00 38.09 .00 33.99 .00 37.32 .00 36.74 .00 37.32 .00 31.05 .00 31.56 .00 30.70 .00 30.03 .00 29.66 .00 30.03 .00 29.66 .00 30.03 .00 29.66 .00 30.03 .00 39.39 .00 39.39 .00 40.78 .00 40.78 .00 40.78 .00 40.78 .00 40.78	
ATOM	.00 33.99 .00 37.32 .00 36.74 .00 36.74 .00 31.05 .00 31.05 .00 31.05 .00 30.70 .00 30.70 .00 30.70 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 30.90 .00 40.70 .00 40.70 .00 40.36 .00 40.36 .00 40.71 .00 40.04 .00 36.89	
S	.00 37.32 .00 36.74 .00 33.52 .00 31.05 .00 31.56 .00 30.70 .00 30.03 .00 29.66 .00 37.90 .00 38.47 .00 39.39 .00 40.78 .00 40.78 .00 40.78 .00 40.78 .00 40.36 .00 40.36 .00 40.36 .00 40.36 .00 40.04 .00 36.89	
ATOM	.00 36.74 .00 31.52 .00 31.56 .00 31.56 .00 31.56 .00 30.70 .00 30.03 .00 29.66 .00 37.90 .00 39.52 .00 39.52 .00 39.39 .00 40.78 .00 40.78 .00 40.78 .00 40.56 .00 40.56 .00 40.56 .00 40.56 .00 40.56 .00 40.56 .00 40.68	
ATOM	.00 33.52 .00 31.56 .00 31.56 .00 31.56 .00 30.70 .00 30.70 .00 30.03 .00 29.66 .00 30.97 .00 38.47 .00 39.52 .00 39.39 .00 40.78 .00 40.78 .00 40.78 .00 40.78 .00 40.36 .00 40.36 .00 40.36 .00 40.36 .00 40.36 .00 40.36	
ATOM	.00 31.05 .00 31.56 .00 30.70 .00 30.03 .00 29.66 .00 37.90 .00 38.47 .00 39.52 .00 39.39 .00 41.43 .00 40.78 .00 45.25 .00 40.56 .00 40.56 .00 40.71	000000000000000000
NATION 2499 C13 GLC G 2 37.712 -6.417 -6.552 1.	.00 31.56 .00 30.70 .00 30.03 .00 29.66 .00 38.47 .00 39.52 .00 39.52 .00 41.43 .00 40.56 .00 40.56 .00 40.71 .00 40.04 .00 36.89	00000000000000000
10	.00 30.70 .00 30.70 .00 30.03 .03 .00 .00 .00 .00 .00 .00	0000000000000000
ATOM	.00 30.03 .00 29.66 .00 37.90 .00 38.47 .00 39.52 .00 39.39 .00 41.43 .00 40.78 .00 40.78 .00 40.36 .00 40.36 .00 40.36	00000000000000
ATOM	.00 29.66 .00 37.90 .00 38.47 .00 39.52 .00 39.39 .00 41.43 .00 40.78 .00 45.25 .00 40.56 .00 40.36 .00 40.71 .00 40.04	0000000000000
ATOM	.00 37.90 .00 38.47 .00 39.52 .00 39.39 .00 41.43 .00 40.78 .00 45.25 .00 40.56 .00 40.71 .00 40.04 .00 40.04	00000000000
ATOM	.00 38.47 .00 39.52 .00 39.39 .00 41.43 .00 40.78 .00 45.25 .00 40.56 .00 40.71 .00 40.04 .00 40.04	00000000000
15	.00 39.52 .00 39.39 .00 41.43 .00 40.78 .00 45.25 .00 40.56 .00 40.36 .00 40.71 .00 40.04 .00 36.89	000000000
ATOM	.00 39.39 .00 41.43 .00 40.78 .00 45.25 .00 40.56 .00 40.36 .00 40.71 .00 40.04 .00 36.89	00000000
ATOM	.00 41.43 .00 40.78 .00 45.25 .00 40.56 .00 40.36 .00 40.71 .00 40.04 .00 36.89	0000000
ATOM	.00 40.78 .00 45.25 .00 40.56 .00 40.36 .00 40.71 .00 40.04 .00 36.89	99999
ATOM	.00 45.25 .00 40.56 .00 40.36 .00 40.71 .00 40.04 .00 36.89	9999
No. No.	.00 45.25 .00 40.56 .00 40.36 .00 40.71 .00 40.04 .00 36.89	9999
20	.00 40.56 .00 40.36 .00 40.71 .00 40.04 .00 36.89	9 9 9
ATOM	.00 40.36 .00 40.71 .00 40.04 .00 36.89	G G
ATOM	.00 40.71 .00 40.04 .00 36.89	G G
ATOM	.00 40.04 .00 36.89	G
ATOM	.00 36.89	
25		G
ATOM		
ATOM	.00 63.04	G
ATOM	.00 62.46	G
ATOM 2519 C15 GLC G G G G G G G G G	.00 61.14	G
30	.00 61.72	G
ATOM	.00 60.51	G
ATOM	.00 58.61	G
ATOM	.00 73.45	G
ATOM	.00 72.78	G
35	.00 72.98	G
ATOM	.00 73.88	G
ATOM	.00 73.66	G
ATOM 2528 C11 GLC G 8 52.447 20.871 5.063 1. ATOM 2530 014 GLC G 8 51.476 20.597 3.098 1. ATOM 2530 014 GLC G 8 51.476 20.597 3.098 1. ATOM 2531 015 GLC G 8 50.1297 21.794 3.150 1. ATOM 2532 016 GLC G 8 50.1297 21.794 3.150 1. ATOM 2533 012 GLC G 10 35.044 37.499 29.523 1. ATOM 2534 011 GLC G 10 35.164 37.499 29.523 1. ATOM 2535 013 GLC G 10 33.649 36.645 30.259 1. ATOM 2536 014 GLC G 10 33.249 36.645 30.259 1. ATOM 2536 014 GLC G 10 33.249 37.772 29.308 1. ATOM 2537 015 GLC G 10 33.249 35.7772 29.308 1. ATOM 2538 016 GLC G 10 33.249 35.542 29.557 1.	.00 75.38	G
ATOM	.00 62.51	G
ATOM	.00 63.42	G
40 ATOM 2530 014 GLC G 8 51.297 21.794 3.150 1. ATOM 2531 015 GLC G 8 50.121 20.137 4.448 1. ATOM 2532 016 GLC G 8 49.233 19.866 3.357 1. ATOM 2534 012 GLC G 10 36.044 37.499 29.523 1. ATOM 2535 013 GLC G 10 35.164 36.645 30.259 1. ATOM 2535 013 GLC G 10 33.249 36.489 29.494 1. ATOM 2536 014 GLC G 10 33.248 37.772 29.308 1. ATOM 2537 015 GLC G 10 33.248 37.772 29.308 1. ATOM 2538 016 GLC G 10 31.674 35.442 29.557 1.	.00 64.28	G
ATOM	.00 66.28	G
ATOM 2532 016 GLC 6 8 49.233 19.866 3.357 1. ATOM 2533 012 GLC 6 10 36.044 37.499 29.523 1. ATOM 2534 011 GLC 6 10 35.164 36.645 30.259 1. ATOM 2535 013 GLC 6 10 33.849 36.645 29.454 1. ATOM 2536 014 GLC G 10 33.248 37.772 29.308 1. ATOM 2537 015 GLC 6 10 32.900 35.560 30.277 1. ATOM 2538 016 GLC 6 10 31.674 35.442 29.557 1.	.00 64.49	G
ATOM 2533 012 GLC G 10 36.044 37.499 29.523 1. ATOM 2534 011 GLC G 10 35.164 36.645 30.259 1. ATOM 2535 013 GLC G 10 33.849 36.469 29.494 1. ATOM 2536 014 GLC G 10 33.848 37.772 29.308 1. ATOM 2537 015 GLC G 10 32.900 35.580 30.277 1. ATOM 2538 016 GLC G 10 31.674 35.442 29.557 1.		G
A TOM 2534 C11 GLC G 10 35.164 36.465 30.259 1. 45 ATOM 2535 C13 GLC G 10 33.649 36.489 29.494 1. ATOM 2536 014 GLC G 10 33.248 37.772 29.308 1. ATOM 2537 015 GLC G 10 32.900 35.580 30.277 1. ATOM 2538 016 GLC G 10 31.674 35.442 29.557 1.		G
45 ATOM 2535 C13 GLC G 10 33.849 36.489 29.494 1. ATOM 2536 014 GLC G 10 33.248 37.772 29.308 1. ATOM 2537 C15 GLC G 10 32.900 35.580 30.277 1. ATOM 2538 016 GLC G 10 31.674 35.442 29.557 1.	.00 64.01	G
ATOM 2536 014 GLC G 10 33.248 37.772 29.308 1. ATOM 2537 C15 GLC G 10 32.900 35.580 30.277 1. ATOM 2538 016 GLC G 10 31.674 35.442 29.557 1.	.00 56.89	
ATOM 2537 C15 GLC G 10 32.900 35.580 30.277 1. ATOM 2538 016 GLC G 10 31.674 35.442 29.557 1.	.00 56.89 .00 56.97	G
ATOM 2538 016 GLC G 10 31.674 35.442 29.557 1.	.00 56.89 .00 56.97 .00 56.11	
	.00 56.89 .00 56.97 .00 56.11 .00 56.44	G
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84	G
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84	G G
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49	G G N
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49	G G N
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41	G G N N
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41	G G N
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41 .00 52.07	G G N N
55 ATOM 2545 O1B ATP N 1 43.083 22.898 3.669 1.	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41 .00 52.07 .00 51.01	G N N N
ATOM 2546 02B ATP N 1 45.345 22.474 4.766 1.	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41 .00 52.07	G N N N N
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41 .00 52.07 .00 51.01	G N N N N
	.00 56.89 .00 56.97 .00 56.11 .00 56.44 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41 .00 52.07 .00 51.01	G N N N N N
ATOM 2549 OLA ATP N 1 45.547 20.291 0.754 1.	.00 56.89 .00 56.97 .00 56.11 .00 56.41 .00 55.84 .00 55.39 .00 51.49 .00 52.22 .00 51.41 .00 52.07 .00 51.01 .00 50.20 .00 49.41	G N N N N N

	ATOM	2550	02A	ATP	N	1	45.807	20.035	3.270	1.00	45.03	N
	ATOM	2551	05*	ATP	N	1	43.516	20.223	2.245	1.00	41.73	N
	ATOM	2552	C5*	ATP	N	1	42.528	20.925	1.489	1.00	37.57	N
	ATOM	2553	C4*	ATP		1	41.127	20.379	1.776		39.45	N
5	ATOM	2554		ATP		1	40.907	19.024	1.279		37.72	N
-	ATOM	2555		ATP		1	40.777	20.321	3.251		38.48	N
	ATOM	2556	03*	ATP	N	î	40.360	21.615	3.697		40.42	N
	ATOM	2557	C2*	ATP		1	39.608	19.374	3.270		37.58	N
	ATOM	2558		ATP		1	38.410	20.076	2.924		35.98	
10												N
10	ATOM	2559		ATP		1	39.939	18.346	2.173		35.55	N
	MOTA	2560	N9	ATP	N	1	40.628	17.156	2.747		31.76	N
	MOTA	2561	C8	ATP		1	41.864	17.126	3.274		30.49	N
	MOTA	2562	N7	ATP		1	42.143	15.877	3.667		29.75	N
	MOTA	2563	C5	ATP		1	41.088	15.118	3.390		27.49	N
15	MOTA	2564	C4	ATP	Ν	1	40.125	15.925	2.810		30.02	N
	MOTA	2565	N3	ATP		1	38.937	15.389	2.431		27.11	N
	MOTA	2566	C2	ATP	N	1	38.679	14.085	2.615		25.62	N
	MOTA	2567	N1	ATP	N	1	39.597	13.283	3.175	1.00	21.76	N
	MOTA	2568	C6	ATP	N	1	40.800	13.768	3.571	1.00	23.90	N
20	MOTA	2569	N6	ATP	N	1	41.698	12.964	4.127	1.00	21.94	N
	MOTA	2570	S	SO4	Ι	1	58.680	8.493	-0.639	1.00	56.05	I
	MOTA	2571	01	SO4	I	1	57.956	7.875	0.483	1.00	58.83	I
	ATOM	2572	02	SO4	I	1	57.886	9.607	-1.188	1.00	57.04	I
	ATOM	2573	03	SO4	Ι	1	58.906	7.478	-1.683	1.00	57.47	I
25	ATOM	2574	04	SO4		1	59.976	9.008	-0.156		57.51	I
	ATOM	2575	S	SO4		2	39.339	4.855	7.057		84.24	Ī
	MOTA	2576	01	SO4		2	39.390	6.175	7.711		85.02	I
	ATOM	2577	02	SO4		2	40.101	4.897	5.797		84.75	Ĩ
	ATOM	2578	03	SO4		2	37.936	4.506	6.766		84.94	Ī
30	ATOM	2579	04	SO4		2	39.931	3.842	7.954		84.44	Ī
30	ATOM	2580	S	SO4		3	38.987	-2.256	3.310		58.58	Ī
	ATOM	2581	01	SO4		3	37.734	-1.675	3.827		59.11	Ī
	ATOM	2582	02	SO4		3	39.460	-1.454	2.172		59.11	Ī
	ATOM	2583	03	SO4		3	38.743	-3.640	2.172		60.97	Ī
25												
35	MOTA	2584	04	SO4		3	40.014	-2.260	4.369		59.58	I
	MOTA	2585	S	SO4		4	34.397	5.289	30.981		64.34	I
	MOTA	2586	01	SO4		4	33.627	6.528	30.742		60.43	I
	MOTA	2587	02	SO4		4	34.337	4.427	29.782		60.11	I
	MOTA	2588	03	SO4		4	33.816	4.572	32.133		64.39	I
40	MOTA	2589	04	SO4		4	35.806	5.626	31.277		63.55	I
	MOTA	2590	S	SO4		5	55.074	-6.984	-3.711		75.40	I
	MOTA	2591	01	SO4		5	54.657	-7.518	-2.399		74.66	I
	MOTA	2592	02	SO4		5	54.209	-5.845	-4.065		74.96	I
	MOTA	2593	03	SO4	Ι	5	54.950	-8.034	-4.742	1.00	74.22	I
45	MOTA	2594	04	SO4	I	5	56.477	-6.532	-3.633	1.00	75.15	I
	MOTA	2595	02	PO4	P	100	57.362	24.998	13.149	1.00	66.76	P
	MOTA	2596	03	PO4	P	100	59.399	26.166	13.761	1.00	66.89	P
	MOTA	2597	04	PO4	P	100	57.761	25.606	15.462	1.00	67.43	P
	ATOM	2598	01	PO4	P	100	57.264	27.325	13.818	1.00	65.91	P
50	ATOM	2599	P			100	57.947	26.025	14.048		66.69	P
	ATOM	2600	СВ	GLU		80	50.411		-13.538		23.31	AC2
	ATOM	2601	CG	GLU		80	51.306		-14.362		24.09	AC2
	ATOM	2602	CD	GLU		80	52.180		-13.509		25.31	AC2
	ATOM	2602		GLU		80	52.841		-12.580		22.80	AC2
55	ATOM	2604		GLU		80	52.212		-13.774		28.07	AC2
23	ATOM	2604	CB	SER		105	37.582	-1.281	-6.192		21.16	AC2
	ATOM		OG	SER			37.127	-1.281	-6.192		20.42	
		2606 2607	CB			105						AC2
	ATOM			ARG		116	59.520	22.977	-7.867		31.00	AC2
	ATOM	2608	CG	ARG		116	60.312	24.192	-8.323	0.50	32.50	AC2

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2609 CD ARG
    ATOM
                        116
                                60.266 24.349 -9.838 0.50 34.11
                                                                     AC2
    MOTA
                                61.045 25.499 -10.290 0.50 36.67
          2610 NE
                  ARG
                        116
                                                                     AC2
    MOTA
          2611
               CZ
                   ARG
                        116
                                60.729 26.766 -10.035 0.50 37.26
                                                                     AC2
          2612 NH1 ARG
                        116
                                59.642 27.053 -9.331 0.50 38.99
                                                                     AC2
    MOTA
                                61.503 27.746 -10.479 0.50 37.83
    MOTA
          2613 NH2 ARG
                        116
                                                                     AC2
    MOTA
          2614 CB LEU
                        145
                                49.693
                                        8.642
                                               6.631 0.50 15.29
                                                                     AC2
                                50.783
                                        8.664
                                                5.552 0.50 14.29
                                                                     AC2
    MOTA
          2615 CG
                   LEU
                        145
                                50.264
                                               4.305 0.50 8.20
    MOTA
          2616 CD1 LEU
                        145
                                        9.373
                                                                     AC2
                                52.030
                                        9.361
    MOTA
          2617
               CD2 LEU
                        145
                                               6.087 0.50 10.66
                                                                     AC2
                                27,455 16,155 24,989 0,50 19,21
    MOTA
          2618 CB ARG
                        183
                                                                     AC2
    MOTA
          2619 CG
                  ARG
                        183
                                28.077 15.397 26.147 0.50 18.46
                                                                     AC2
    ATOM
          2620 CD
                  ARG
                        183
                                27.002
                                       14.945 27.127
                                                      0.50 19.72
                                                                     AC2
                                26.016 14.086
    MOTA
          2621 NE
                   ARG
                        183
                                               26.478 0.50 18.79
                                                                     AC2
                                24.703 14.279
          2622 CZ
                        183
                                               26.539 0.50 18.52
    MOTA
                  ARG
                                                                     AC2
                                24.213 15.305 27.221 0.50 15.35
          2623 NH1 ARG
                        183
    MOTA
                                                                     AC2
          2624 NH2 ARG
                        183
                               23.881 13.445 25.915 0.50 17.55
    MOTA
                                                                     AC2
                        191
                               38.479 10.847 23.036 0.50 16.57
    MOTA
          2625 CB SER
                                                                     AC2
                               37.418 10.765 23.973 0.50 18.62
    ATOM
          2626 OG SER
                        191
                                                                     AC2
                        209
                                38.645 24.079
                                               8.551 0.50 22.02
    ATOM
          2627 CB GLU
                                                                     AC2
                                37.769 25.296
                                               8.263 0.50 23.40
    MOTA
          2628 CG GLU
                        209
                                                                     AC2
                                37.513 26.175
    MOTA
          2629 CD GLU
                        209
                                               9.483 0.50 24.27
                                                                     AC2
                               37.076 27.328
    MOTA
          2630 OE1 GLU
                        209
                                               9.288 0.50 25.25
                                                                     AC2
    MOTA
          2631 OE2 GLU
                        209
                               37.737 25.727 10.629 0.50 20.24
                                                                     AC2
                               38.598 32.546 14.790 0.50 18.71
    MOTA
          2632 CB GLN
                        247
                                                                     AC2
                               38.077 33.665 13.900 0.50 16.95
2.5
    MOTA
          2633 CG GLN
                       247
                                                                     AC2
                               38.614 33.598 12.479 0.50 19.13
          2634 CD GLN
                        247
                                                                     AC2
    MOTA
                               39.763 33.221 12.246 0.50 17.24
          2635 OE1 GLN 247
                                                                     AC2
    MOTA
          2636 NE2 GLN 247
                               37.780 33.979 11.520 0.50 19.88
                                                                     AC2
    MOTA
          2637 CE LYS 315
                               34.978 25.150 36.369 0.50 20.49
                                                                     AC2
    MOTA
30
    MOTA
          2638 NZ LYS
                        315
                               34.183 24.074 37.023 0.50 17.05
                                                                     AC2
         2639 CB GLN 352
                               32.365 1.170 19.731 0.50 31.10
    MOTA
                                                                     AC2
    ATOM 2640 CG GLN 352
                               33.833 0.778 19.683 0.50 32.11
                                                                     AC2
                               34.190 0.027 18.419 0.50 33.04
         2641 CD GLN 352
                                                                     AC2
    MOTA
                             33.906 0.485 17.314 0.50 34.87
         2642 OE1 GLN 352
    MOTA
                                                                     AC2
35
         2643 NE2 GLN 352
                               34.819 -1.133 18.575 0.50 32.08
    MOTA
                                                                     AC2
    END
```

Example 3: Co-ordinates for the PDK1 fragment without alternate side chains.

40

```
REMARK coordinates from restrained individual B-factor refinement
 REMARK refinement resolution: 25.0 - 2.0 A
 REMARK starting r= 0.1972 free r= 0.2220
REMARK final
               r= 0.1954 free r= 0.2224
REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5
 REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
REMARK rweight= 0.0900 (with wa= 1.29263)
REMARK target= mlf steps= 30
REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
gamma= 120
 REMARK parameter file 1 : /ddl/david/projects/PDK1 new/CNS/prot.par
REMARK parameter file 2 : /ddl/david/projects/PDKl new/CNS/atp.par
REMARK parameter file 3 : CNS TOPPAR:water rep.param
REMARK parameter file 4 : CNS TOPPAR:ion.param
```

```
REMARK parameter file 5 : /dd1/david/projects/PDK1 new/CNS/glycerol.par
    REMARK molecular structure file: ../generate/alternate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../1/hkl/cns.hkl
5 REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.0
    REMARK initial B-factor correction applied to fobs :
    REMARK B11= -2.766 B22= -2.766 B33= 5.532
REMARK B12= -0.375 B13= 0.000 B23= 0.000
10 REMARK B-factor correction applied to coordinate array B: 0.031
    REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
    REMARK reflections with |Fobs|/sigma F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range: 28210 ( 100.0
    REMARK number of unobserved reflections (no entry or |F|=0): 568 (
                                                                      2.0
    8 )
    REMARK number of reflections rejected:
                                                                0 (
                                                                    0.0
    % )
    REMARK total number of reflections used:
                                                             27642 ( 98.0
    8 )
    REMARK number of reflections in working set:
                                                             27063 ( 95.9
    9. 1
                                                              579 ( 2.1
    REMARK number of reflections in test set:
2.5
   9. 1
    CRYST1 123.013 123.013 47.624 90.00 90.00 120.00 P 32 2 1
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE: 16-Apr-2002 18:31:12
                                      created by user: david
    REMARK VERSION: 1.0
30
  ATOM
            1 CB PRO A 71
                                58.912 -7.251 8.216 1.00 67.78
    MOTA
             2 CG PRO A 71
                                59.621 -6.941 9.534 1.00 69.16
    MOTA
             3 C PRO A 71
                                59.493 -6.506 5.894 1.00 67.06
            4 O PRO A 71
                                59.196 -5.318 5.766 1.00 66.66
    MOTA
            5 N PRO A 71
                                60.984 -6.073 7.833 1.00 67.86
    MOTA
35 ATOM
                                60.554 -5.762 9.207 1.00 68.24
            6 CD PRO A 71
            7 CA PRO A 71
                                60.040 -7.035 7.217 1.00 67.75
    MOTA
    ATOM
            8 N PRO A 72
                                59.356 -7.385 4.890 1.00 66.32
    ATOM
            9 CD PRO A 72
                                59.712 -8.816 4.898 1.00 67.17
    ATOM
           10 CA PRO A 72
                                58.840 -6.986 3.578 1.00 65.61
   MOTA
           11 CB PRO A 72
                                58.672 -8.321 2.858 1.00 66.47
    MOTA
           12 CG PRO A 72
                               59.796 -9.133 3.419 1.00 67.57
    MOTA
           13 C PRO A 72
                                57.527 -6.208 3.673 1.00 63.94
                                                                     A
           14 O PRO A 72
                                56.710 -6.451
                                               4.561 1.00 64.11
    MOTA
                                                                     A
    MOTA
           15 N ALA A 73
                                57.341 -5.268
                                                2.753 1.00 61.57
                                                                     Α
           16 CA ALA A 73
                                56.133 -4.454 2.708 1.00 58.74
   MOTA
                                                                     Α
    MOTA
           17 CB ALA A 73
                                56.438 -3.030 3.165 1.00 58.05
                                                                     Α
    ATOM
           18 C
                   ALA A 73
                                55.626 -4.448 1.271 1.00 56.78
                                                                     Α
    ATOM
           19 O ALA A 73
                                56.347 -4.834 0.349 1.00 56.95
    ATOM
           20 N PRO A 74
                                54.372 -4.024 1.057 1.00 54.15
                                                                     Α
   ATOM
           21 CD PRO A 74
                                53.335 -3.610 2.018 1.00 53.31
                                                                     Α
    ATOM
           22 CA PRO A 74
                                53.856 -4.003 -0.314 1.00 52.54
    ATOM
           23 CB PRO A 74
                                52.474
                                        -3.375 -0.148 1.00 52.86
                                                                     Α
    MOTA
           24 CG PRO A 74
                                52.067
                                        -3.824
                                               1.226 1.00 52.88
                                                                     А
           25 C
                   PRO A 74
                                54.772
                                        -3.167 -1.204 1.00 50.08
    MOTA
                                                                     Α
           26 O
                  PRO A 74
                                55.559
                                        -2.361 -0.708 1.00 49.96
   ATOM
                                                                     А
    MOTA
           27 N
                   ALA A 75
                                54.680 -3.366 -2.514 1.00 47.58
                                                                     Α
           28 CA ALA A 75
                                55.503 -2.602 -3.446 1.00 44.69
    MOTA
                                                                     Λ
           29 CB ALA A 75
                               55.312 -3.121 -4.870 1.00 46.14
    MOTA
           30 C ALA A 75
                               55.100 -1.134 -3.371 1.00 41.55
    ATOM
```

	ATOM	31	0	ALA	Α	75	53.947	-0.813	-3.086	1.00	41.01	A
	ATOM	32	N	LYS		76	56.053	-0.245	-3.619		38.31	A
	ATOM	33	CA	LYS		76	55.781	1.184	-3.588		35.72	A
	ATOM	34	CB	LYS		76	57.053	1.957	-3.930		37.70	A
5	ATOM	35	CG	LYS		76	57.123	3.356	-3.350		40.99	A
,	ATOM	36	CD	LYS		76	57.262	3.316	-1.836		40.04	A
	ATOM	37	CE	LYS		76	57.511	4.705	-1.277		42.08	A
	ATOM	38	NZ	LYS		76	57.681	4.695	0.202		42.99	A
	ATOM	39	С	LYS		76	54.708	1.467	-4.638		32.65	A
10	MOTA	40	0	LYS		76	54.814	1.005	-5.770		31.41	A
	ATOM	41	N		Α	77	53.668	2.207	-4.270		28.59	A
	ATOM	42	CA	LYS		77	52.619	2.517	-5.232		25.72	A
	ATOM	43	CB	LYS	Α	77	51.316	2.865	-4.509	1.00	26.22	A
	MOTA	44	CG	LYS	Α	77	50.796	1.731	-3.631	1.00	27.15	A
15	ATOM	45	CD	LYS	Α	77	49.487	2.089	-2.967	1.00	26.80	A
	ATOM	46	CE	LYS	A	77	49.136	1.091	-1.870	1.00	27.31	A
	ATOM	47	NZ	LYS	А	77	48.998	-0.296	-2.380	1.00	27.17	A
	ATOM	48	С	LYS		77	53.053	3.668	-6.137	1.00	24.67	A
	ATOM	49	ō		A	77	54.010	4.377	-5.829		21.60	A
20	ATOM	50	N	ARG		78	52.351	3.838	-7.254		23.66	A
20	ATOM	51	CA	ARG		78	52.662	4.897	-8.211		26.14	A
	ATOM	52	CB	ARG		78	53.574	4.344	-9.318		28.57	A
		53				78						
	MOTA		CG	ARG			53.017		-10.050		34.78	A
	MOTA	54	CD	ARG		78	54.092		-10.896		40.96	A
25	MOTA	55	NE	ARG		78	53.560		-11.700		48.93	A
	MOTA	56	CZ	ARG		78	52.985		-11.203		52.58	A
	MOTA	57		ARG		78	52.860	0.113	-9.889		54.60	A
	ATOM	58		ARG		78	52.530		-12.022		54.09	A
	ATOM	59	C	ARG	Α	78	51.382	5.488	-8.803	1.00	23.76	A
30	MOTA	60	0	ARG	Α	78	50.311	4.888	-8.706	1.00	24.25	A
	ATOM	61	N	PRO	Α	79	51.475	6.676	-9.428	1.00	21.76	A
	ATOM	62	CD	PRO	Α	79	52.691	7.475	-9.668	1.00	20.82	A
	ATOM	63	CA	PRO	Α	79	50.301	7.325	-10.021	1.00	21.96	A
	ATOM	64	CB	PRO	А	79	50.910	8.481	-10.816	1.00	22.27	A
35	ATOM	65	CG	PRO	A	79	52.124	8.831	-10.014	1.00	22.12	A
	ATOM	66	C	PRO		79	49.446		-10.903		22.86	A
	ATOM	67	o	PRO		79	48.213		-10.842		20.52	A
	ATOM	68	N	GLU		80	50.103		-11.714		21.87	A
	ATOM	69	CA	GLU		80	49.403		-12.628		22.99	A
40	ATOM	70	CB	GLU		80	50.393		-13.571		25.24	A
40												
	MOTA	71	CG	GLU		80	51.230		-12.925		28.75	A
	MOTA	72	CD	GLU		80	52.157		-13.913		31.99	A
	MOTA	73		GLU		80	53.072		-14.433		34.34	A
	MOTA	74		GLU		80	51.969		-14.172		32.83	A
45	MOTA	75	С	GLU		80	48.556		-11.912		22.09	A
	MOTA	76	0	GLU		80	47.692		-12.530		22.37	A
	ATOM	77	N	ASP	Α	81	48.804	3.413	-10.622	1.00	19.97	A
	MOTA	78	CA	ASP	A	81	48.026	2.423	-9.874	1.00	19.93	A
	MOTA	79	CB	ASP	A	81	48.736	2.029	-8.571	1.00	21.19	A
50	ATOM	80	CG	ASP	Α	81	50.089	1.380	-8.807	1.00	22.46	A
	ATOM	81	OD1	ASP	Α	81	50.195	0.554	-9.731	1.00	24.22	A
	ATOM	82		ASP		81	51.043	1.685	-8.058		23.33	A
	ATOM	83	C	ASP		81	46.652	2.975	-9.518		20.85	A
	ATOM	84	ō	ASP		81	45.793	2.246	-9.015		19.96	A
55	ATOM	85	N	PHE		82	46.445	4.258	-9.804		18.91	A
22	ATOM	86	CA	PHE		82	45.200	4.238	-9.465		19.30	A
	ATOM	86	CB	PHE		82		6.027	-8.427		18.43	A
							45.475					
	MOTA	88	CG	PHE		82	46.134	5.531	-7.175		18.01	A
	MOTA	89	CD1	PHE	Α	82	45.371	5.136	-6.084	1.00	17.19	A

	MOTA	90		PHE		82	47.520	5.460	-7.086	1.00 18.99	A
	MOTA	91	CE1	PHE	A	82	45.977	4.676	-4.918	1.00 17.12	A
	ATOM	92	CE2	PHE	Α	82	48.137	5.000	-5.925	1.00 19.64	A
	ATOM	93	CZ	PHE	A	82	47.361	4.607	-4.838	1.00 18.00	A
5	ATOM	94	C	PHE		82	44.476		-10.621	1.00 20.81	A
,											
	MOTA	95	0	PHE		82	45.066		-11.649	1.00 20.34	A
	ATOM	96	N	LYS		83	43.182		-10.411	1.00 19.80	A
	MOTA	97	CA	LYS	A	83	42.321	6.478	-11.353	1.00 21.65	A
	ATOM	98	CB	LYS	A	83	41.096	5.625	-11.687	1.00 22.02	A
10	ATOM	99	CG	LYS	A	83	40.062	6.326	-12.550	1.00 28.93	A
	ATOM	100	CD	LYS	А	83	38.974	5.355	-12.981	1.00 34.20	A
	ATOM	101	CE	LYS	A	83	37.909		-13.824	1.00 38.10	A
	ATOM	102	NZ	LYS		83	37.179		-13.043	1.00 43.33	A
					A	83	41.913		-10.541	1.00 20.74	A
1.5	ATOM	103	С								
15	MOTA	104	0	LYS		83	41.084	7.606	-9.635	1.00 20.98	A
	MOTA	105	N		A	84	42.513		-10.835	1.00 19.99	A
	MOTA	106	CA	PHE	Α	84	42.188	10.049	-10.083	1.00 18.63	A
	MOTA	107	CB	PHE	A	84	43.279	11.103	-10.258	1.00 18.95	A.
	ATOM	108	CG	PHE	Α	84	44.571	10.741	-9.587	1.00 17.68	A
20	ATOM	109	CD1	PHE	Α	84	45.498	9.926	-10.224	1.00 18.16	A
	ATOM	110			A	84	44.843	11.183	-8.299	1.00 19.66	A
	ATOM	111		PHE	A	84	46.676	9.556	-9.589	1.00 18.09	A
		112			A	84	46.021	10.816	-7.653	1.00 18.89	
	ATOM										A
	MOTA	113	CZ	PHE	A	84	46.936	10.002	-8.301	1.00 17.33	A
25	MOTA	114	C	PHE		84	40.834	10.617		1.00 19.69	A
	MOTA	115	0	PHE		84	40.391	10.489	-11.601	1.00 20.72	A
	MOTA	116	N	GLY	A	85	40.178	11.233	-9.484	1.00 16.80	A
	ATOM	117	CA	GLY	A	85	38.872	11.810	-9.716	1.00 17.73	A
	ATOM	118	C	GLY	А	85	38.819	13.280	-9.346	1.00 18.75	A
30	ATOM	119	o	GLY		85	39.740	14.043	-9.650	1.00 18.45	A
	ATOM	120	N	LYS		86	37.753	13.673	-8.659	1.00 16.00	A
	ATOM	121	CA		A	86	37.571	15.064	-8.278	1.00 18.26	A
	ATOM	122	CB	LYS		86	36.133	15.302	-7.812	1.00 10.20	A
	MOTA	123	CG	LYS		86	35.793	14.660	-6.481	1.00 21.55	A
35	MOTA	124	CD	LYS		86	34.368	14.981	-6.066	1.00 26.48	A
	ATOM	125	CE	LYS	Α	86	33.994	14.239	-4.793	1.00 31.92	A.
	MOTA	126	NZ	LYS	A	86	32.568	14.457	-4.412	1.00 35.36	A
	ATOM	127	C	LYS	A	86	38.523	15.571	-7.202	1.00 18.57	A
	ATOM	128	0	LYS	A	86	39.045	14.807	-6.385	1.00 16.77	A
40	ATOM	129	N	ILE	Δ	87	38.737	16.881	-7.227	1.00 17.88	A
	ATOM	130	CA	ILE		87	39.577	17.554	-6.256	1.00 18.26	A
	ATOM	131	CB	ILE		87	39.994	18.952	-6.772	1.00 19.60	A
						87					
	ATOM	132		ILE			40.593	19.786	-5.628	1.00 18.73	A
	MOTA	133		ILE		87	40.968	18.786	-7.945	1.00 21.16	A
45	MOTA	134		ILE		87	41.412	20.087	-8.588	1.00 25.26	A
	MOTA	135	C	ILE	A	87	38.731	17.709	-4.997	1.00 19.67	A.
	MOTA	136	0	ILE	A	87	37.628	18.249	-5.052	1.00 20.41	A
	ATOM	137	N	LEU	A	88	39.240	17.229	-3.867	1.00 19.15	A
	ATOM	138	CA	LEU	A	88	38.508	17.324	-2.611	1.00 20.68	A
50	ATOM	139	CB	LEU		88	38.870	16.151	-1.700	1.00 19.97	A
	ATOM	140	CG	LEU		88	38.529	14.759	-2.237	1.00 19.24	A
	ATOM	141		LEU		88	39.090	13.692	-1.311	1.00 21.41	A
	MOTA	142		LEU		88	37.029	14.622	-2.359	1.00 18.84	A
	MOTA	143	C	LEU		88	38.815	18.632	-1.901	1.00 23.11	A
55	MOTA	144	0	LEU		88	37.999	19.146	-1.139	1.00 25.10	A
	MOTA	145	N	GLY	Α	89	39.997	19.174	-2.149	1.00 24.09	A
	MOTA	146	CA	GLY	Α	89	40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	C	GLY	A	89	41.658	20.954	-2.078	1.00 25.47	A
	ATOM	148	ō	GLY		89	42.445	20.202	-2.666	1.00 22.19	A
				-							

	ATOM	149	**	OT 11		90	41 070	00 054	-1.906	1 00 00 00	
			N	GLU			41.870	22.254		1.00 26.22	A
	MOTA	150	CA	GLU		90	43.064	22.924	-2.404	1.00 29.96	A
	ATOM	151	CB	GLU	Α	90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU	A	90	42.267	23.038	-4.831	1.00 34.32	A
5	ATOM	153	CD	GLU	A	90	41.711	23.930	-5.927	1.00 38.27	A
	ATOM	154		GLU		90	40.590	24.456	-5.764	1.00 40.57	A
	ATOM	155		GLU		90	42.398	24.110	-6.952	1.00 40.90	A
	MOTA	156	C	GLU		90	43.711	23.768	-1.313	1.00 30.68	A
	MOTA	157	0	GLU		90	43.049	24.574	-0.668	1.00 32.83	A
10	MOTA	158	N	GLY		91	45.006	23.566	-1.104	1.00 29.66	A
	MOTA	159	CA	GLY	Α	91	45.724	24.332	-0.104	1.00 29.40	A
	ATOM	160	C	GLY	A	91	46.795	25.151	-0.798	1.00 29.98	A
	ATOM	161	0	GLY	A	91	46.894	25.130	-2.028	1.00 28.16	A
	ATOM	162	N	SER	Α	92	47.605	25.870	-0.029	1.00 28.30	A
15	ATOM	163	CA	SER		92	48.653	26.681	-0.633	1.00 30.50	A
	ATOM	164	CB	SER		92	49.165	27.717	0.370	1.00 32.43	A
	ATOM	165	OG	SER		92	49.520	27.099	1.593	1.00 40.94	A
	ATOM	166		SER		92	49.815	25.843	-1.164	1.00 29.77	A
			С								
	MOTA	167	0	SER		92	50.456	26.221	-2.143	1.00 30.46	A
20	ATOM	168	N	PHE	A	93	50.087	24.703	-0.536	1.00 27.65	A
	ATOM	169	CA	PHE	Α	93	51.185	23.855	-0.995	1.00 26.34	A
	ATOM	170	CB	PHE	A	93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	A	93	52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE	Α	93	52.283	25.909	1.392	1.00 29.96	A
25	ATOM	173	CD2	PHE	A	93	53.949	25.613	-0.308	1.00 31.38	A
	ATOM	174	CE1	PHE	A	93	52.779	27.181	1.665	1.00 32.69	A
	ATOM	175	CE2		A	93	54.452	26.883	-0.044	1.00 32.63	A
	ATOM	176	CZ	PHE	A	93	53.864	27.670	0.945	1.00 32.03	A
	MOTA	177	С	PHE		93	50.759	22.445	-1.365	1.00 25.39	A
30	MOTA	178	0	PHE		93	51.601	21.559	-1.522	1.00 24.59	A
	ATOM	179	N	SER		94	49.457	22.235	-1.519	1.00 23.63	A
	MOTA	180	CA	SER	Α	94	48.965	20.912	-1.860	1.00 21.43	A
	ATOM	181	CB	SER	A	94	49.017	20.013	-0.628	1.00 21.42	A
	ATOM	182	OG	SER	A	94	48.091	20.475	0.340	1.00 21.19	A
35	ATOM	183	С	SER	А	94	47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	o	SER		94	46.795	21.882	-2.173	1.00 18.76	A
	ATOM	185	N	THR		95	47.174	19.832	-3.038	1.00 19.38	A
	ATOM	186	CA	THR		95	45.840	19.637	-3.580	1.00 17.98	A
	ATOM	187	CB	THR		95	45.818	19.818	-5.110	1.00 17.30	A
40											
40	MOTA	188		THR		95	46.196	21.162	-5.434	1.00 22.04	A
	MOTA	189		THR		95	44.421	19.549	-5.661	1.00 17.61	A
	MOTA	190	C	THR		95	45.455	18.201	-3.243	1.00 18.61	A
	ATOM	191	0	THR		95	46.212	17.264	-3.524	1.00 17.10	A
	MOTA	192	N	VAL	A	96	44.295	18.024	-2.623	1.00 16.53	A
45	ATOM	193	CA	VAL	A	96	43.845	16.685	-2.266	1.00 16.05	A
	ATOM	194	CB	VAL	A	96	43.170	16.672	-0.886	1.00 16.32	A
	ATOM	195		VAL		96	42.741	15.249	-0.532	1.00 18.02	A
	ATOM	196		VAL		96	44.145	17.206	0.168	1.00 16.69	A
	ATOM	197	c	VAL		96	42.875	16.207	-3.335	1.00 16.42	A
50	ATOM	198	0	VAL		96	41.906	16.892	-3.665	1.00 16.42	A
50											
	MOTA	199	N	VAL		97	43.157	15.033	-3.888	1.00 16.80	A
	MOTA	200	CA	VAL		97	42.338	14.471	-4.949	1.00 16.72	A
	MOTA	201	CB	VAL		97	43.153	14.354	-6.255	1.00 18.43	A
	MOTA	202		VAL		97	42.249	13.927	-7.404	1.00 19.69	A
55	MOTA	203	CG2	VAL	Α	97	43.831	15.685	-6.569	1.00 17.84	A
	ATOM	204	C	VAL	A	97	41.812	13.091	-4.583	1.00 16.77	A
	ATOM	205	0	VAL	Α	97	42.532	12.270	-4.014	1.00 17.13	A
	ATOM	206	N	LEU		98	40.545	12.845	-4.895	1.00 16.62	A
	ATOM	207	CA	LEU		98	39.947	11.548	-4.624	1.00 17.04	A
	111 011		UN	220	**	50	55.541	11.540	1.027	1.00 17.01	A

	ATOM	208	CB	LEU	А	98	38.424	11.633	-4.743	1.00 16.89	A
	ATOM	209	CG	LEU		98	37,635	10.342	-4.508	1.00 19.46	A
	ATOM	210		LEU		98	37.990	9.762	-3.146	1.00 20.07	A
	ATOM	211		LEU		98	36.143	10.627	-4.588	1.00 17.93	A
5	ATOM	212	C	LEU		98	40.512	10.597	-5.677	1.00 17.38	A
	ATOM	213	ō	LEU		98	40.527	10.920	-6.863	1.00 18.60	A
	ATOM	214	N	ALA		99	40.995	9.438	-5.246	1.00 17.13	A
	ATOM	215	CA	ALA		99	41.570	8.466	-6.168	1.00 17.13	A
	ATOM	216	CB	ALA		99	43.090	8.524	-6.105	1.00 14.76	A
10						99		7.055		1.00 14.76	
10	ATOM	217	C	ALA			41.102		-5.848		A
	MOTA	218	0	ALA		99	40.941	6.691	-4.679	1.00 22.52	A
	MOTA	219	N	ARG			40.878	6.261	-6.888	1.00 19.77	A
	MOTA	220	CA	ARG			40.459	4.884	-6.693	1.00 20.85	A
	MOTA	221	CB			100	39.202	4.585	-7.518	1.00 24.22	A
15	MOTA	222	CG	ARG			38.608	3.205	-7.256	1.00 31.78	A
	ATOM	223	CD	ARG			37.326	2.979	-8.048	1.00 36.24	A
	MOTA	224	NE			100	36.213	3.818	-7.594	1.00 41.40	A
	MOTA	225	CZ			100	35.566	3.662	-6.439	1.00 42.05	A
	MOTA	226		ARG			35.912	2.696	-5.598	1.00 40.67	A
20	MOTA	227		ARG			34.559	4.468	-6.128	1.00 43.65	A
	MOTA	228	C	ARG	Α	100	41.613	3.985	-7.129	1.00 18.63	A
	MOTA	229	0	ARG	Α	100	42.078	4.065	-8.271	1.00 19.49	A
	MOTA	230	N	GLU	Α	101	42.102	3.157	-6.212	1.00 16.43	A
	ATOM	231	CA	GLU	Α	101	43.196	2.246	-6.533	1.00 16.11	A
25	ATOM	232	CB	GLU	Α	101	43.774	1.637	-5.248	1.00 16.79	A
	ATOM	233	CG	GLU	Α	101	44.917	0.657	-5.488	1.00 16.51	A
	ATOM	234	CD	GLU	Α	101	45.501	0.115	-4.200	1.00 18.20	A
	ATOM	235	OE1	GLU	Α	101	44.733	-0.081	-3.239	1.00 18.32	A
	MOTA	236	OE2	GLU	Α	101	46.725	-0.132	-4.150	1.00 17.14	A
30	MOTA	237	C	GLU	Α	101	42.625	1.152	-7.442	1.00 17.92	A
	ATOM	238	ò			101	41.681	0.462	-7.069	1.00 18.02	A
	ATOM	239	N			102	43.198	1.002	-8.632	1.00 19.06	A
	ATOM	240	CA			102	42.718	0.025	-9.607	1.00 20.71	A
	ATOM	241	CB			102	43.569		-10.878	1.00 23.42	A
35	ATOM	242	CG			102	43.531		-11.642	1.00 25.30	A
	ATOM	243		LEU			44.577		-12.748	1.00 27.88	A
	ATOM	244		LEU			42.140		-12.214	1.00 26.79	A
	ATOM	245	C			102	42.671	-1.418	-9.125	1.00 21.62	A
	ATOM	246	Ö			102	41.668	-2.103	-9.305	1.00 21.02	A
40	ATOM	247	N	ALA			43.753	-1.874	-8.507	1.00 19.38	A
40	ATOM	248	CA	ALA			43.836	-3.249	-8.035	1.00 20.87	A
	ATOM	249	CB	ALA			45.284	-3.571	-7.671	1.00 20.07	A
	ATOM	250	С	ALA			42.919	-3.629	-6.872	1.00 19.23	A
	ATOM	251	0	ALA			42.703	-4.815	-6.628	1.00 20.38	A
45	ATOM	252	N			103	42.763	-2.643	-6.175	1.00 18.12	A
43											
	ATOM	253	CA			104	41.517	-2.927	-5.018	1.00 17.15	A
	ATOM	254	CB			104	42.212	-2.484	-3.717	1.00 19.54	A
	ATOM	255		THR			42.456	-1.070	-3.773	1.00 19.26	A
50	MOTA	256		THR			43.536	-3.219	-3.529	1.00 17.02	A
50	MOTA	257	С			104	40.159	-2.247	-5.026	1.00 19.44	A
	MOTA	258	0			104	39.259	-2.648	-4.285	1.00 18.70	A
	ATOM	259	N			105	40.034	-1.207	-5.847	1.00 19.65	A
	ATOM	260	CA			105	38.819	-0.400	-5.967	1.00 19.37	A
	MOTA	261	CB			105	37.598	-1.304	-6.173	1.00 21.81	A
55	MOTA	262	OG			105	36.431	-0.539	-6.412	1.00 23.01	A
	MOTA	263	C			105	38.644	0.447	-4.701	1.00 18.99	A
	MOTA	264	0			105	37.602	1.070	-4.488	1.00 18.66	A
	ATOM	265	N			106	39.674	0.468	-3.861	1.00 16.84	A
	ATOM	266	CA	ARG	Α	106	39.655	1.267	-2.634	1.00 16.21	A

	MOTA	267	CB	ARG	Α	106	40.827	0.886	-1.723	1.00 16		A
	MOTA	268	CG	ARG	Α	106	40.619	-0.367	-0.906	1.00 15		A
	MOTA	269	CD	ARG	Α	106	41.887	-0.755	-0.170	1.00 17	.43	A
	ATOM	270	NE	ARG	Α	106	41.620	-1.792	0.824	1.00 20	. 47	A
5	ATOM	271	CZ	ARG	Α	106	42.548	-2.568	1.371	1.00 20	.24	A
	MOTA	272	NH1	ARG	Α	106	43.821	-2.433	1.017	1.00 17	.80	A
	ATOM	273	NH2	ARG	Α	106	42.198	-3.468	2.285	1.00 20	.14	A
	ATOM	274	C	ARG	Α	106	39.785	2.746	-2.981	1.00 17	.37	A
	ATOM	275	0	ARG	Α	106	40.514	3.103	-3.902	1.00 17	.75	A
10	ATOM	276	N	GLU	Α	107	39.085	3.599	-2.240	1.00 16	.06	A
	ATOM	277	CA	GLU	Α	107	39.156	5.039	-2.461	1.00 20	.80	A
	ATOM	278	CB			107	37.779	5.694	-2.337	1.00 22		A
	ATOM	279	CG	GLU	Α	107	36.711	5.171	-3.269	1.00 30	.87	A
	ATOM	280	CD	GLU	Α	107	35.431	5.975	-3.148	1.00 32	.40	A
15	ATOM	281	OE1	GLU	Α	107	35.262	6.939	-3.923	1.00 33	.74	A
	ATOM	282	OE2	GLU	Α	107	34.608	5.654	-2.263	1.00 36	.00	A
	ATOM	283	C	GLU	Α	107	40.053	5.678	-1.410	1.00 18	.93	A
	ATOM	284	0			107	39.891	5.427	-0.220	1.00 19		A
	ATOM	285	N			108	40.988	6.507	-1.852	1.00 16		A
20	ATOM	286	CA	TYR	Α	108	41.883	7.209	-0.942	1.00 15	.86	A
	ATOM	287	CB	TYR	Α	108	43.325	6.728	-1.104	1.00 15	.30	A
	ATOM	288	CG	TYR	Α	108	43.593	5.328	-0.612	1.00 16	.33	А
	ATOM	289	CD1	TYR	А	108	43.765	5.066	0.746	1.00 16	.36	A
	ATOM	290	CE1				44.046	3.769	1.201	1.00 18		A
25	ATOM	291	CD2	TYR			43.701	4.268	-1.511	1.00 13		A
	ATOM	292	CE2	TYR	Α	108	43.980	2.981	-1.075	1.00 17	.28	A
	ATOM	293	CZ	TYR	Α	108	44.152	2.736	0.276	1.00 19	.17	А
	ATOM	294	OH	TYR	Α	108	44.440	1.461	0.688	1.00 19	.38	A
	ATOM	295	С	TYR	Α	108	41.850	8.687	-1.292	1.00 16	.80	A
30	ATOM	296	0	TYR	Α	108	41.560	9.058	-2.431	1.00 15	.22	A
	ATOM	297	N	ALA	Α	109	42.132	9.528	-0.306	1.00 14	.61	A
	ATOM	298	CA	ALA	Α	109	42.207	10.957	-0.539	1.00 14	.30	A
	ATOM	299	CB	ALA	Α	109	41.671	11.726	0.661	1.00 14	.78	A
	ATOM	300	C	ALA	Α	109	43.713	11.136	-0.667	1.00 16	.79	A
35	ATOM	301	0	ALA	Α	109	44.450	10.983	0.317	1.00 16	.52	A
	ATOM	302	N	ILE	Α	110	44.182	11.410	-1.881	1.00 14	.80	A
	ATOM	303	CA	ILE	Α	110	45.609	11.574	-2.093	1.00 15	.80	A
	ATOM	304	CB	ILE	Α	110	46.065	10.863	-3.396	1.00 16	.85	A
	MOTA	305	CG2	ILE	Α	110	47.550	11.098	-3.632	1.00 16	.80	A
40	MOTA	306	CG1	ILE	Α	110	45.774	9.358	-3.284	1.00 17	.76	A
	ATOM	307	CD1	ILE	Α	110	46.308	8.513	-4.437	1.00 16	.07	A
	MOTA	308	С	ILE	Α	110	46.004	13.045	-2.129	1.00 17	.78	A
	ATOM	309	0	ILE	Α	110	45.534	13.813	-2.976	1.00 16	.24	A
	MOTA	310	N	LYS	Α	111	46.846	13.435	-1.177	1.00 16	.15	A
45	MOTA	311	CA	LYS	Α	111	47.326	14.808	-1.100	1.00 17	.20	A
	MOTA	312	CB	LYS	Α	111	47.700	15.176	0.344	1.00 17	.41	A
	ATOM	313	CG	LYS	Α	111	48.350	16.547	0.464	1.00 20	.71	A
	MOTA	314	CD	LYS	Α	111	48.585	16.971	1.910	1.00 24	.25	A
	MOTA	315	CE	LYS	Α	111	47.288	17.381	2.598	1.00 29	.46	A
50	ATOM	316	NZ	LYS	Α	111	47.516	17.866	4.000	1.00 30	.50	A
	MOTA	317	C	LYS	Α	111	48.551	14.890	-1.994	1.00 16	.41	A
	MOTA	318	0	LYS	Α	111	49.509	14.137	-1.813	1.00 18	.20	A
	ATOM	319	N	ILE	Α	112	48.509	15.798	-2.963	1.00 15	.87	A
	MOTA	320	CA	ILE	Α	112	49.606	15.967	-3.907	1.00 17	.28	A
55	MOTA	321	CB	ILE	Α	112	49.079	15.911	-5.358	1.00 16	.43	A
	ATOM	322	CG2	ILE	Α	112	50.235	15.998	-6.341	1.00 15	.12	A
	MOTA	323	CG1				48.293	14.609	-5.565	1.00 16	.82	A
	MOTA	324	CD1	ILE			47.580	14.511	-6.904	1.00 18		A
	MOTA	325	C	ILE	Α	112	50.307	17.301	-3.663	1.00 19	.03	A

	ATOM	326	0	ILE	А	112	49.669	18.350	-3.635	1.00 19.15	A
	ATOM	327	N	LEU			51.622	17.245	-3.472	1.00 20.22	A
	ATOM	328	CA	LEU			52.416	18.442	-3.214	1.00 22.36	A
	ATOM	329	CB	LEU			52.995	18.397	-1.794	1.00 22.30	A
5	ATOM	330	CG	LEU			52.042	18.063	-0.646	1.00 22.15	A
,	ATOM	331		LEU			51.866	16.557	-0.553	1.00 23.81	A
	ATOM	332		LEU			52.603	18.595	0.660	1.00 23.68	A
	ATOM	333	C	LEU			53.560	18.547	-4.215	1.00 23.37	A
10	ATOM	334	0	LEU			54.300	17.586	-4.424	1.00 23.11	A
10	MOTA	335	N	GLU			53.706	19.714	-4.834	1.00 23.88	A
	MOTA	336	CA	GLU			54.771	19.920	-5.806	1.00 26.00	A
	ATOM	337	CB	GLU			54.435	21.111	-6.706	1.00 27.74	A
	MOTA	338	CG	GLU			55.533	21.452	-7.696	1.00 35.07	A
	ATOM	339	CD	GLU			55.220	22.696	-8.497	1.00 39.24	A
15	MOTA	340		GLU			54.808	23.703	-7.885	1.00 41.45	A
	ATOM	341	OE2	GLU	Α	114	55.395	22.670	-9.736	1.00 44.05	A.
	MOTA	342	C	GLU	Α	114	56.087	20.163	-5.067	1.00 24.37	A
	ATOM	343	0	GLU	Α	114	56.186	21.071	-4.238	1.00 24.43	A
	ATOM	344	N	LYS	Α	115	57.096	19.350	-5.360	1.00 24.10	A
20	ATOM	345	CA	LYS	Α	115	58.376	19.493	-4.678	1.00 24.93	A
	ATOM	346	CB	LYS	Α	115	59.339	18.373	-5.103	1.00 23.72	A
	ATOM	347	CG	LYS	А	115	59.139	17.080	-4.308	1.00 23.09	A
	ATOM	348	CD	LYS			60.064	15.944	-4.743	1.00 21.92	A
	ATOM	349	CE	LYS			59.691	15.400	-6.117	1.00 22.42	A
25	ATOM	350	NZ	LYS			60.447	14.150	-6.448	1.00 19.71	A
	ATOM	351	C	LYS			59.031	20.858	-4.868	1.00 26.87	A
	ATOM	352	Ö	LYS			59.492	21.469	-3.903	1.00 26.17	A
	ATOM	353	N	ARG			59.058	21.348	-6.102	1.00 28.73	A
	ATOM	354	CA	ARG			59.678	22.638	-6.380	1.00 29.66	A
30	ATOM	355	CB	ARG			59.533	22.980	-7.868	1.00 29.66	A
30			CG								
	ATOM	356		ARG			60.047	24.361	-8.267	1.00 33.19	A
	ATOM	357	CD	ARG			61.368	24.710	-7.590	1.00 35.13	A
	ATOM	358	NE	ARG			62.329	23.612	-7.618	1.00 36.42	A
	MOTA	359	CZ	ARG			63.510	23.648	-7.009	1.00 36.18	A
35	MOTA	360		ARG			63.871	24.729	-6.332	1.00 36.12	A
	ATOM	361		ARG			64.324	22.602	-7.067	1.00 35.77	A
	MOTA	362	С	ARG			59.097	23.761	-5.519	1.00 29.70	A
	MOTA	363	0	ARG			59.843	24.515	-4.889	1.00 29.16	A
	MOTA	364	N	HIS			57.773	23.862	-5.472	1.00 27.22	A
40	MOTA	365	CA	HIS			57.126	24.903	-4.681	1.00 26.33	A
	MOTA	366	CB	HIS			55.606	24.835	-4.848	1.00 28.41	A.
	MOTA	367	CG	HIS	Α	117	54.881	26.005	-4.258	1.00 31.82	A
	ATOM	368	CD2	HIS	Α	117	55.309	27.249	-3.935	1.00 33.19	A
	MOTA	369	ND1	HIS	Α	117	53.536	25.974	-3.961	1.00 34.30	A
45	ATOM	370	CE1	HIS	Α	117	53.165	27.148	-3.480	1.00 34.58	A
	ATOM	371	NE2	HIS	Α	117	54.222	27.940	-3.455	1.00 35.18	A
	ATOM	372	С	HIS	А	117	57.477	24.780	-3.202	1.00 26.22	A
	ATOM	373	0	HIS	А	117	57.737	25.776	-2.534	1.00 25.67	A
	ATOM	374	N	ILE			57.469	23.554	-2.689	1.00 24.94	A
50	ATOM	375	CA	ILE			57.792	23.315	-1.285	1.00 23.94	A
	ATOM	376	СВ	ILE			57.711	21.812	-0.952	1.00 23.50	A
	ATOM	377		ILE			58.374	21.533	0.389	1.00 23.76	A
	ATOM	378		ILE			56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379		ILE			56.066	19.858	-0.834	1.00 24.42	A
55	ATOM	380	CDI	ILE				23.821	-0.958	1.00 28.06	A
55							59.195				
	ATOM	381	0	ILE			59.402	24.495	0.048	1.00 23.49	A
	ATOM	382	N	ILE			60.153	23.489	-1.815	1.00 23.46	A
	ATOM	383	CA	ILE			61.534	23.913	-1.619	1.00 25.13	A
	MOTA	384	CB	ILE	Α	119	62.467	23.250	-2.664	1.00 24.25	A

	ATOM	385	CG2	ILE	А	119	63.858	23.890	-2.617	1.00 22.47	/ A
	ATOM	386	CG1	ILE	А	119	62.540	21.738	-2.395	1.00 25.05	5 A
	ATOM	387		ILE			63.327	20.945	-3.439	1.00 24.62	
	ATOM	388	c			119	61.667	25.435	-1.705	1.00 25.96	
5	ATOM	389	ō			119	62,330	26.051	-0.872	1.00 24.78	
-	ATOM	390	N			120	61.028	26.039	-2.704	1.00 27.67	
	ATOM	391	CA			120	61.100	27.489	-2.879	1.00 30.29	
	ATOM	392	CB			120	60.242	27.940	-4.060	1.00 30.23	
	ATOM	393	CG			120	60.242	27.407	-5.409	1.00 32.3	
10											
10	ATOM	394	CD			120	59.765	27.950	-6.512	1.00 45.19	
	ATOM	395	CE			120	58.294	27.636	-6.218	1.00 46.48	
	ATOM	396	NZ			120	57.363	28.155	-7.252	1.00 46.49	
	MOTA	397	C			120	60.647	28.247	-1.638	1.00 30.89	
	MOTA	398	0			120	61.303	29.198	-1.217	1.00 32.48	
15	MOTA	399	N			121	59.527	27.825	-1.055	1.00 29.82	
	MOTA	400	CA			121	58.986	28.488	0.128	1.00 30.33	
	ATOM	401	CB	GLU	Α	121	57.455	28.416	0.117	1.00 33.04	
	MOTA	402	CG	GLU	Α	121	56.794	29.021	-1.120	1.00 36.45	5 A
	MOTA	403	CD	GLU	Α	121	57.221	30.456	-1.373	1.00 39.88	3 A
20	MOTA	404	OE1	GLU	Α	121	57.200	31.264	-0.420	1.00 40.53	3 A
	ATOM	405	OE2	GLU	Α	121	57.573	30.778	-2.529	1.00 43.24	l A
	ATOM	406	C	GLU	Α	121	59.511	27.930	1.451	1.00 30.37	/ A
	ATOM	407	0	GLU	Α	121	58.946	28.204	2.513	1.00 31.24	A I
	MOTA	408	N	ASN	Α	122	60.588	27.151	1.390	1.00 29.03	3 A
25	ATOM	409	CA	ASN			61.183	26.573	2.594	1.00 28.46	
	ATOM	410	CB	ASN			61.836	27.673	3.436	1.00 31.28	
	ATOM	411	CG	ASN			62.945	28.395	2.698	1.00 34.12	
	ATOM	412		ASN			62.697	29.143	1.754	1.00 35.57	
	ATOM	413		ASN			64.181	28.169	3.127	1.00 35.73	
30	ATOM	414	C			122	60.157	25.835	3.456	1.00 26.89	
50	ATOM	415	Ö			122	60.085	26.055	4.663	1.00 27.23	
	ATOM	416				123	59.375	24.955	2.842	1.00 27.23	
	ATOM	417	N CA			123	58.358	24.933		1.00 23.99	
									3.574		
2.5	MOTA	418	CB	LYS			57.031	24.248	2.810	1.00 21.97	
35	ATOM	419	CG			123	56.475	25.645	2.599	1.00 25.68	
	ATOM	420	CD			123	56.253	26.354	3.927	1.00 27.54	
	MOTA	421	CE			123	55.822	27.796	3.716	1.00 31.30	
	MOTA	422	NZ			123	55.756	28.540	5.004	1.00 33.21	
	MOTA	423	C			123	58.748	22.759	3.821	1.00 22.20	
40	MOTA	424	0			123	57.924	21.960	4.264	1.00 22.50	
	MOTA	425	N			124	59.997	22.412	3.535	1.00 20.59	
	ATOM	426	CA			124	60.439	21.039	3.730	1.00 20.25	
	ATOM	427	CB	VAL	Α	124	61.922	20.850	3.328	1.00 19.43	3 A
	MOTA	428	CG1	VAL	Α	124	62.346	19.407	3.573	1.00 18.69	A (
45	MOTA	429	CG2	VAL	Α	124	62.104	21.195	1.853	1.00 18.21	L A
	ATOM	430	C	VAL	Α	124	60.236	20.561	5.163	1.00 19.53	3 A
	ATOM	431	0	VAL	Α	124	59.841	19.418	5.385	1.00 20.02	. A
	ATOM	432	N	PRO	Α	125	60.513	21.422	6.159	1.00 20.01	L A
	ATOM	433	CD			125	61.178	22.738	6.118	1.00 18.69	
50	ATOM	434	CA			125	60.318	20.979	7.544	1.00 19.88	
	ATOM	435	СВ			125	60.793	22.180	8.363	1.00 19.95	
	ATOM	436	CG			125	61.839	22.805	7.479	1.00 18.85	
	ATOM	437	c			125	58.848	20.642	7.824	1.00 19.76	
	ATOM	438	0			125	58.544	19.700	8.550	1.00 16.99	
55	ATOM	439	N			126	57.947	21.418	7.235	1.00 18.98	
55	ATOM	440	CA			126			7.435	1.00 18.98	
							56.516	21.220			
	MOTA	441	CB			126	55.752	22.448	6.933	1.00 25.17	
	MOTA	442	CG			126	56.040	23.690	7.748	1.00 30.98	
	ATOM	443	CD1	TYR	Α	126	55.438	23.886	8.991	1.00 33.95	5 A

	ATOM	444	CE1	TYR	Α	126	55.721	25.015	9.763	1.00	36.60	A
	ATOM	445	CD2	TYR	Α	126	56.938	24.657	7.292	1.00	35.43	A
	ATOM	446	CE2	TYR			57.231	25.792	8.058		37.20	A
	ATOM	447	CZ	TYR			56.618	25.962	9.291		37.40	A
-												
5	MOTA	448	OH	TYR			56.903	27.073	10.052		40.85	A
	MOTA	449	C	TYR			55.990	19.956	6.762		21.35	A
	ATOM	450	0	TYR	Α	126	55.265	19.175	7.383	1.00	20.49	A
	ATOM	451	N	VAL	Α	127	56.354	19.746	5.501	1.00	18.16	A
	ATOM	452	CA	VAL	Α	127	55.892	18.562	4.790	1.00	17.58	A
10	ATOM	453	CB	VAL	Α	127	56.308	18.596	3.308	1.00	17.45	A
	ATOM	454	CG1	VAL	А	127	55.786	17.350	2.600	1.00	17.97	A
	ATOM	455	CG2				55.751	19.850	2.641		14.90	A
	ATOM	456	C	VAL			56.459	17.306	5.448		18.39	A
		457	o	VAL			55.769	16.298	5.583		18.14	A
15	ATOM											
15	MOTA	458	N	THR			57.716	17.381	5.869		17.50	A
	MOTA	459	CA	THR			58.375	16.260	6.530		18.54	A
	ATOM	460	CB	THR			59.861	16.586	6.805		18.01	A
	MOTA	461	OG1	THR	Α	128	60.537	16.804	5.559	1.00	21.14	A
	MOTA	462	CG2	THR	Α	128	60.536	15.446	7.545	1.00	17.95	A
20	ATOM	463	C	THR	Α	128	57.676	15.941	7.856	1.00	19.49	A
	ATOM	464	0	THR	Α	128	57.438	14.776	8.179	1.00	18.76	A
	ATOM	465	N	ARG			57.345	16.981	8.619		19.60	A
	ATOM	466	CA	ARG			56.673	16.804	9.904		20.12	A
	ATOM	467	CB	ARG			56.534	18.144	10.621		21.33	A
25	ATOM	468	CG	ARG			55.948	18.029	12.023		28.02	A
23												
	ATOM	469	CD	ARG			55.721	19.404	12.597		31.25	A
	MOTA	470	NE	ARG			56.940	20.205	12.560		37.78	A
	MOTA	471	CZ	ARG			56.962	21.524	12.391		40.10	A
	MOTA	472		ARG			55.828	22.197	12.239		40.03	A
30	ATOM	473	NH2	ARG	Α	129	58.119	22.170	12.374	1.00	44.58	A
	ATOM	474	C	ARG	Α	129	55.288	16.186	9.729	1.00	20.08	A
	ATOM	475	0	ARG	Α	129	54.891	15.305	10.496	1.00	20.40	A
	ATOM	476	N	GLU			54.553	16.654	8.724		18.79	A
	ATOM	477	CA	GLU			53.222	16.125	8.454		20.10	A
35	ATOM	478	CB	GLU			52.638	16.749	7.183		19.92	A
33	ATOM	479	CG	GLU			51.350	16.087	6.708		27.85	A
		480	CD	GLU								
	ATOM						50.581	16.933	5.707		29.72	A
	MOTA	481		GLU			51.216	17.528	4.814		33.46	A
	MOTA	482		GLU			49.339	16.996	5.807		30.74	A
40	MOTA	483	C	GLU			53.301	14.615	8.295		19.81	A
	MOTA	484	0	GLU	Α	130	52.553	13.875	8.935	1.00	18.37	A.
	ATOM	485	N	ARG	Α	131	54.219	14.162	7.447	1.00	20.41	A
	ATOM	486	CA	ARG	Α	131	54.397	12.735	7.202	1.00	22.45	A
	ATOM	487	CB	ARG	Α	131	55.442	12.511	6.098	1.00	25.16	A
45	ATOM	488	CG	ARG	Α	131	55.742	11.043	5.840	1.00	28.75	A
	ATOM	489	CD	ARG			56.736	10.837	4.708		33.75	A
	ATOM	490	NE	ARG			57.020	9.415	4.520		40.07	A
	ATOM	491	CZ	ARG			57.756	8.915	3.532		43.07	A
50	MOTA	492		ARG			58.293	9.721	2.625		44.91	A
50	MOTA	493		ARG			57.955	7.606	3.449		44.45	A
	MOTA	494	C	ARG			54.820	11.982	8.466		23.24	A
	ATOM	495	0	ARG			54.241	10.948	8.804		23.86	A
	MOTA	496	N	ASP	Α	132	55.831	12.497	9.160	1.00	21.99	A
	ATOM	497	CA	ASP	Α	132	56.318	11.850	10.370	1.00	22.04	A
55	ATOM	498	CB	ASP	Α	132	57.570	12.564	10.888	1.00	23.72	A
	ATOM	499	CG	ASP	Α	132	58.750	12.442	9.932	1.00	27.77	A
	ATOM	500		ASP			58.681	11.620	8.989		27.34	A
	ATOM	501		ASP			59.753	13.163	10.128		28.70	A
	ATOM	502	C	ASP			55.258	11.772	11.474		21.69	A
	ALUM	302	C	MDP	м	132	JJ. ZJ8	11.112	11.4/4	1.00	21.09	A

	MOTA	503	0	ASP			55.077	10.723	12.092		22.75	A
	ATOM	504	N	VAL	Α	133	54.551	12.868	11.725	1.00	19.54	A
	ATOM	505	CA	VAL	Α	133	53.525	12.843	12.759	1.00	18.52	A
	ATOM	506	CB	VAL	А	133	52.908	14.244	12.990	1.00	19.26	A
5	ATOM	507		VAL			51.708	14.135	13.918		18.79	A
	ATOM	508		VAL				15.180	13.604			
							53.953				18.80	A
	MOTA	509	C	VAL			52.419	11.854	12.398		19.46	A
	MOTA	510	0	VAL			52.073	10.991	13.200		19.94	A
	MOTA	511	N	MET			51.878	11.957	11.187		19.15	A
10	ATOM	512	CA	MET	Α	134	50.807	11.052	10.792	1.00	21.25	A
	ATOM	513	CB	MET	Α	134	50.309	11.381	9.383	1.00	17.34	A
	ATOM	514	CG	MET	А	134	49.615	12.730	9.302	1.00	20.00	A
	ATOM	515	SD	MET			48.643	12.952	7.798		24.21	A
	ATOM	516	CE	MET			47.033	12.434	8.400		23.20	A
15	ATOM	517	C	MET			51.203	9.582	10.881		22.43	A
13												
	MOTA	518	0	MET			50.384	8.741	11.249		23.82	A
	MOTA	519	N	SER			52.454	9.273	10.556		23.09	A
	MOTA	520	CA	SER			52.939	7.895	10.615		26.13	A
	MOTA	521	CB	SER	Α	135	54.356	7.798	10.039		26.17	A
20	ATOM	522	OG	SER	Α	135	54.383	8.177	8.673	1.00	31.91	A
	ATOM	523	C	SER	Α	135	52.957	7.358	12.045	1.00	26.58	A
	ATOM	524	0	SER	А	135	52,926	6.148	12,261	1.00	26.42	A
	ATOM	525	N	ARG			53.014	8.261	13.018		25.65	A
	ATOM	526	CA	ARG			53.056	7.870	14.425		27.47	A
25	ATOM	527	CB	ARG			53.823	8.914	15.238		27.97	A
23		528		ARG			55.283	9.082	14.857			
	MOTA		CG								32.00	A
	MOTA	529	CD	ARG			55.904	10.218	15.664		33.03	A
	MOTA	530	NE	ARG			55.602	10.073	17.084		36.11	A
	ATOM	531	CZ	ARG			55.867	10.990	18.007	1.00	39.74	A
30	ATOM	532	NH1	ARG	Α	136	56.449	12.132	17.661	1.00	40.55	A
	ATOM	533	NH2	ARG	Α	136	55.540	10.769	19.276	1.00	36.72	A
	ATOM	534	С	ARG	А	136	51.667	7.709	15.036	1.00	26.38	A
	ATOM	535	ō	ARG			51.516	7.121	16.106		27.06	A
	ATOM	536	N	LEU			50.655	8.235	14.360		24.77	A
35	ATOM	537	CA	LEU			49.294	8.162	14.870		24.70	A
33												
	MOTA	538	CB	LEU			48.483	9.363	14.371		24.52	A
	MOTA	539	CG	LEU			49.050	10.760	14.662		26.67	A
	MOTA	540		LEU			48.075	11.813	14.141		27.25	A
	MOTA	541	CD2	LEU			49.279	10.945	16.155		27.09	A
40	MOTA	542	C	LEU	Α	137	48.592	6.868	14.473	1.00	25.20	A
	ATOM	543	0	LEU	Α	137	48.619	6.469	13.309	1.00	25.99	A
	ATOM	544	N	ASP	Α	138	47.971	6.218	15.451	1.00	21.89	A
	ATOM	545	CA	ASP	Α	138	47.239	4.977	15.219	1.00	21.35	A
	ATOM	546	CB	ASP			48.124	3.761	15.523		22.14	A
45	ATOM	547	CG	ASP			47.432	2.448	15.201		24.90	A
75	ATOM	548		ASP			46.631	2.423	14.241		24.78	A
				ASP					15.897			
	MOTA	549					47.691	1.443			25.39	A
	MOTA	550	C	ASP			46.031	4.991	16.138		20.47	A
	MOTA	551	0	ASP			45.967	4.248	17.118		19.06	A
50	MOTA	552	N	HIS	Α	139	45.075	5.852	15.810	1.00	18.27	A
	ATOM	553	CA	HIS	Α	139	43.869	6.016	16.606	1.00	18.21	A
	ATOM	554	CB	HIS	Α	139	44.096	7.157	17.612	1.00	15.84	A
	ATOM	555	CG	HIS	А	139	42.985	7.332	18,600	1.00	15.24	A
	ATOM	556	CD2	HIS	А	139	42.884	6.964	19.900	1.00	13.97	A
55	ATOM	557		HIS			41.791	7.943	18.280		14.74	A
22	ATOM	558		HIS			41.002	7.944	19.341		14.19	A
	MOTA	559		HIS			41.641	7.356	20.336		14.15	A
	MOTA	560	C	HIS			42.715	6.330	15.654		18.50	A
	MOTA	561	0	HIS	Α	139	42.879	7.080	14.693	1.00	20.80	A

	ATOM	562	N	PRO	А	140	41.527	5.767	15.913	1.00 18.32	A
	ATOM	563	CD			140	41.143	4.984	17.100	1.00 16.71	
	ATOM	564	CA	PRO			40.367	6.001	15.048	1.00 17.43	
	ATOM	565	CB	PRO			39.273	5.157	15.704	1.00 16.64	
5	ATOM	566	CG	PRO			39.643	5.204	17.152	1.00 18.43	
,	ATOM	567	c	PRO			39.914	7.441	14.803	1.00 18.77	
	ATOM	568	Ö	PRO			39.207	7.695	13.831	1.00 19.88	
	ATOM	569	N	PHE			40.301	8.381	15.664	1.00 17.14	
	ATOM	570	CA	PHE			39.874	9.767	15.477	1.00 16.42	
10	MOTA	571	CB	PHE			39.568	10.422	16.836	1.00 14.60	
	ATOM	572	CG	PHE			38.386	9.817	17.556	1.00 15.26	
	ATOM	573	CD1	PHE	Α	141	37.335	9.234	16.842	1.00 14.78	A
	MOTA	574	CD2	PHE	Α	141	38.297	9.880	18.942	1.00 13.70	A
	ATOM	575	CE1	PHE	Α	141	36.215	8.727	17.502	1.00 16.94	A
15	ATOM	576	CE2	PHE	Α	141	37.178	9.375	19.615	1.00 15.75	A
	ATOM	577	CZ	PHE	Α	141	36.135	8.799	18.893	1.00 16.89	A
	MOTA	578	С	PHE	А	141	40.857	10.641	14.694	1.00 16.15	A
	ATOM	579	0	PHE	А	141	40.799	11.871	14.761	1.00 17.35	
	ATOM	580	N	PHE			41.748	10.011	13.941	1.00 15.88	
20	ATOM	581	CA	PHE			42.727	10.756	13.154	1.00 17.89	
20	ATOM	582	CB	PHE			44.115	10.645	13.793	1.00 17.57	
	ATOM	583	CG	PHE			44.240	11.371	15.103	1.00 18.74	
		584									
	MOTA			PHE			44.559	12.726	15.135	1.00 17.77	A
	MOTA	585		PHE			43.997	10.711	16.304	1.00 18.74	A
25	MOTA	586		PHE			44.632	13.417	16.347	1.00 15.77	A
	MOTA	587		PHE			44.065	11.393	17.522	1.00 17.56	
	MOTA	588	CZ	PHE			44.383	12.747	17.542	1.00 17.14	
	ATOM	589	C	PHE			42.793	10.231	11.729	1.00 19.12	A
	ATOM	590	0	PHE	Α	142	42.659	9.030	11.504	1.00 20.01	. A
30	MOTA	591	N	VAL	Α	143	42.978	11.135	10.769	1.00 18.72	A
	ATOM	592	CA	VAL	Α	143	43.102	10.735	9.371	1.00 18.52	A
	ATOM	593	CB	VAL	Α	143	43.294	11.961	8.440	1.00 20.66	A
	ATOM	594	CG1	VAL	А	143	43.843	11.521	7.080	1.00 21.29	
	ATOM	595	CG2	VAL	А	143	41.958	12.673	8.252	1.00 22.97	A
35	ATOM	596	С	VAL			44.342	9.865	9.330	1.00 18.68	
	ATOM	597	ō	VAL			45.355	10.199	9.943	1.00 18.42	
	ATOM	598	N	LYS			44.259	8.745	8.623	1.00 18.30	
	ATOM	599	CA	LYS			45.384	7.824	8.535	1.00 18.78	
	ATOM	600	CB	LYS			44.889	6.373	8.608	1.00 22.27	A
40								5.340			
40	ATOM	601	CG	LYS			46.017		8.557	1.00 29.72	
	MOTA	602	CD	LYS			45.491	3.912	8.674	1.00 34.16	
	MOTA	603	CE	LYS			46.631	2.896	8.577	1.00 37.67	
	MOTA	604	NZ	LYS			46.138	1.484	8.629	1.00 39.02	
	MOTA	605	C	LYS			46.192	8.002	7.261	1.00 18.53	
45	MOTA	606	0	LYS	Α	144	45.643	8.314	6.200	1.00 18.18	A
	ATOM	607	N	LEU	Α	145	47.502	7.816	7.385	1.00 16.79	A
	ATOM	608	CA	LEU	Α	145	48.411	7.900	6.251	1.00 17.45	A
	ATOM	609	CB	LEU	Α	145	49.686	8.653	6.641	1.00 18.82	A
	MOTA	610	CG	LEU	А	145	50.734	8.902	5.549	1.00 20.23	
50	MOTA	611		LEU			51.836	9.799	6.093	1.00 18.83	
	ATOM	612		LEU			51.317	7.581	5.069	1.00 19.79	
	ATOM	613	C	LEU			48.739	6.450	5.907	1.00 19.19	
	ATOM	614	ŏ	LEU			49.451	5.772	6.659	1.00 17.36	
	ATOM	615	N	TYR			48.215	5.772	4.782	1.00 17.36	
55											
23	MOTA	616	CA	TYR			48.444	4.593	4.358	1.00 17.57	A
	MOTA	617	CB	TYR			47.288	4.098	3.486	1.00 17.74	
	MOTA	618	CG	TYR			45.981	3.926	4.214	1.00 17.50	
	MOTA	619		TYR			45.099	4.995	4.377	1.00 16.50	
	ATOM	620	CE1	TYR	Α	146	43.881	4.827	5.039	1.00 17.10	A

	MOTA	621	CD2	TYR	Α	146	45.620	2.686	4.735	1.00 1	3.28	Α
	ATOM	622	CE2	TYR	Α	146	44.411	2.506	5.399	1.00 1	9.84	Α
	ATOM	623	CZ	TYR			43.547	3.576	5.544	1.00 1		Α
	MOTA	624	OH	TYR			42.342	3.376	6.169	1.00 20		Α
5	MOTA	625	C	TYR	Α	146	49.735	4.376	3.582	1.00 1	3.72	Α
	ATOM	626	0	TYR	Α	146	50.382	3.338	3.715	1.00 1	9.51	Α
	ATOM	627	N	PHE	Δ	147	50.110	5.350	2.765	1.00 1		Α
	ATOM	628	CA	PHE			51.307	5.203	1.952	1.00 1		A
	ATOM	629	CB	PHE			51.007	4.258	0.783	1.00 1		А
10	MOTA	630	CG	PHE			49.835	4.699	-0.070	1.00 1		А
	MOTA	631	CD1	PHE	Α	147	49.967	5.752	-0.975	1.00 1	5.58	Α
	ATOM	632	CD2	PHE	А	147	48.595	4.075	0.053	1.00 1	3.07	Α
	ATOM	633		PHE			48.886	6.178	-1.742	1.00 1		А
			CE2	PHE			47.503	4.492	-0.710	1.00 1		A
	ATOM	634										
15	MOTA	635	CZ	PHE			47.647	5.546	-1.610	1.00 1		А
	ATOM	636	C	PHE			51.768	6.533	1.395	1.00 1		Α
	ATOM	637	0	PHE	Α	147	51.045	7.528	1.452	1.00 1	4.43	Α
	ATOM	638	N	THR	А	148	52.981	6.534	0.854	1.00 1	7.12	А
	ATOM	639	CA	THR			53.541	7.718	0.232	1.00 1		A
20												
20	MOTA	640	CB	THR			54.449	8.531	1.197	1.00 2		A
	ATOM	641	OG1	THR	Α	148	55.605	7.760	1.537	1.00 1	3.83	А
	ATOM	642	CG2	THR	Α	148	53.700	8.897	2.472	1.00 1	9.60	Α
	ATOM	643	C	THR	Α	148	54.386	7.262	-0.946	1.00 20	0.31	Α
	ATOM	644	0	THR			54.860	6.124	-0.991	1.00 1	9.4	А
25	ATOM	645	N	PHE			54.543	8.149	-1.916	1.00 1		A
23												
	MOTA	646	CA	PHE			55.368	7.877	-3.073	1.00 1		A
	ATOM	647	CB	PHE	Α	149	54.748	6.801	-3.989	1.00 1	7.23	Α
	MOTA	648	CG	PHE	Α	149	53.389	7.144	-4.544	1.00 1	5.88	Α
	MOTA	649	CD1	PHE	Α	149	53.262	7.888	-5.712	1.00 18	3.58	Α
30	ATOM	650	CD2	PHE	Δ	149	52.235	6.668	-3.927	1.00 1		А
50	ATOM	651	CE1	PHE			52.233	8.149	-6.267	1.00 1		A
	MOTA	652	CE2	PHE			50.972	6.923	-4.470	1.00 1		А
	ATOM	653	CZ	PHE	Α	149	50.858	7.663	-5.642	1.00 1	9.60	Α
	ATOM	654	C	PHE	Α	149	55.542	9.205	-3.774	1.00 20	0.85	Α
35	ATOM	655	0	PHE	А	149	54.934	10.200	-3.376	1.00 1	9.76	Α
	ATOM	656	N	GLN			56.398	9.241	-4.782	1.00 1		A
	MOTA	657	CA	GLN			56.636	10.481	-5.497	1.00 2		A
	MOTA	658	CB	GLN			57.659	11.347	-4.739	1.00 2		Α
	ATOM	659	CG	GLN	Α	150	58.986	10.645	-4.414	1.00 2	5.28	Α
40	ATOM	660	CD	GLN	Α	150	59.988	11.558	-3.692	1.00 2	9.02	Α
	MOTA	661	OE1	GLN	А	150	60.693	12.353	-4.321	1.00 2	7.05	А
	ATOM	662		GLN			60.042	11.449	-2.365	1.00 2		Α
	ATOM	663	C	GLN			57.160	10.203	-6.885	1.00 2		A
	MOTA	664	0	GLN			57.673	9.118	-7.158	1.00 2		Α
45	ATOM	665	N	ASP	Α	151	56.987	11.171	-7.774	1.00 2	5.88	Α
	ATOM	666	CA	ASP	Α	151	57.527	11.047	-9.117	1.00 2	5.49	Α
	ATOM	667	CB	ASP	Δ	151	56.437	11.126	-10.199	1.00 2	4.54	Α
	ATOM	668	CG	ASP			55.544		-10.064	1.00 2		A
	ATOM	669		ASP			56.005	13.379	-9.561	1.00 2		A
50	MOTA	670	OD2	ASP	Α	151	54.369		-10.490	1.00 2	5.72	А
	MOTA	671	C	ASP	Α	151	58.515	12.203	-9.220	1.00 2	3.63	Α
	MOTA	672	0	ASP	Α	151	58.890	12.780	-8.194	1.00 2	7.83	Α
	ATOM	673	N	ASP			58.934		-10.426	1.00 2		А
	ATOM	674	CA	ASP			59.907		-10.562	1.00 3		A
55	ATOM	675	CB	ASP			60.325		-12.026	1.00 3		A
	MOTA	676	CG	ASP			61.033		-12.557	1.00 3		Α
	ATOM	677	OD1	ASP	Α	152	61.817	11.959	-11.791	1.00 3	9.67	Α
	ATOM	678	OD2	ASP	Α	152	60.817	12.211	-13.738	1.00 43	1.57	Α
	ATOM	679	C	ASP			59.487		-10.013	1.00 3		A
	111011	373	_	AU E	n	102	55.407	14.554	20.013	1.00 3		n

	ATOM	680	0	ASP	70	152	60.316	15.735	-9.482	1.00 3	1 60	Α
	ATOM	681	N	GLU			58.207		-10.107	1.00 2		A
		682		GLU			57.767	16.632	-9.646	1.00 2		A
	ATOM		CA									
_	MOTA	683	CB	GLU			56.984		-10.766	1.00 3		A
5	MOTA	684	CG	GLU			57.451		-12.183	1.00 4		А
	MOTA	685	CD	GLU			56.920		-12.675	1.00 4		Α
	ATOM	686		GLU			55.682		-12.760	1.00 4		Α
	MOTA	687	OE2	GLU	Α	153	57.736	14.747	-12.979	1.00 4	8.95	Α
	MOTA	688	C	GLU	Α	153	56.929	16.683	-8.372	1.00 2	6.43	Α
10	ATOM	689	0	GLU	Α	153	56.947	17.688	-7.660	1.00 2	5.08	Α
	ATOM	690	N	LYS	Α	154	56.205	15.610	-8.069	1.00 2	2.39	Α
	ATOM	691	CA	LYS	Α	154	55.318	15.631	-6.912	1.00 2	1.43	Α
	MOTA	692	CB	LYS			53.861	15.628	-7.398	1.00 2	0.33	Α
	ATOM	693	CG	LYS	А	154	53.505	16.716	-8.403	1.00 2		Α
15	ATOM	694	CD	LYS			52.211	16.375	-9.146	1.00 1		А
	ATOM	695	CE	LYS			51.775		-10.077	1.00 2		A
	ATOM	696	NZ	LYS			50.631	17.094		1.00 1		A
	ATOM	697	C	LYS			55.458	14.522	-5.881	1.00 2		Α
	ATOM	698	Ö	LYS			55.949	13.426	-6.173	1.00 2		A
20	ATOM	699	N	LEU			54.985	14.832	-4.676	1.00 1		А
20									-3.553			
	ATOM	700	CA	LEU			54.950	13.900		1.00 1		A
	ATOM	701	CB	LEU			55.362	14.588	-2.252	1.00 1		Α
	ATOM	702	CG	LEU			56.740	15.234	-2.129	1.00 2		A
	MOTA	703		LEU			56.848	15.918	-0.770	1.00 2		A
25	MOTA	704		LEU			57.816	14.174	-2.277	1.00 2		A
	ATOM	705	C	LEU			53.478	13.507	-3.427	1.00 1		А
	ATOM	706	0	LEU	Α	155	52.600	14.348	-3.620	1.00 1	8.61	Α
	ATOM	707	N	TYR			53.209	12.249	-3.091	1.00 1		Α
	MOTA	708	CA	TYR	Α	156	51.834	11.783	-2.934	1.00 1	6.29	Α
30	MOTA	709	CB	TYR	Α	156	51.470	10.769	-4.029	1.00 1	4.20	Α
	ATOM	710	CG	TYR	Α	156	51.603	11.273	-5.449	1.00 1	7.29	Α
	ATOM	711	CD1	TYR	Α	156	52.857	11.429	-6.045	1.00 1	6.46	Α
	ATOM	712	CE1	TYR	Α	156	52.978	11.884	-7.360	1.00 1	8.68	Α
	ATOM	713	CD2	TYR	Α	156	50.474	11.588	-6.202	1.00 1	6.43	Α
35	ATOM	714	CE2	TYR	А	156	50.583	12.048	-7.512	1.00 1		А
	ATOM	715	CZ	TYR			51.835	12.192	-8.083	1.00 1		A
	ATOM	716	OH	TYR			51.941	12.651	-9.371	1.00 1		A
	ATOM	717	C	TYR			51.657	11.108	-1.572	1.00 1		A
	ATOM	718	ō	TYR			52.412	10.197	-1.235	1.00 1		A
40	ATOM	719	N	PHE			50.678	11.568	-0.792	1.00 1		A
40	ATOM	720	CA	PHE			50.385	10.966	0.508	1.00 1		A
	ATOM	721	CB	PHE			50.324	12.014	1.629	1.00 1		A
	ATOM	722	CG	PHE			51.631	12.708	1.907	1.00 1		A
4.5	ATOM	723		PHE			52.821	12.261	1.340	1.00 2		Α
45	ATOM	724		PHE			51.664	13.829	2.732	1.00 2		Α
	MOTA	725		PHE			54.025	12.926	1.585	1.00 2		A
	MOTA	726	CE2	PHE			52.865	14.500	2.982	1.00 2		А
	MOTA	727	CZ	PHE			54.045	14.045	2.405	1.00 2		Α
	MOTA	728	C	PHE			49.016	10.308	0.404	1.00 1		Α
50	MOTA	729	0	PHE			48.029	10.979	0.110	1.00 1		А
	ATOM	730	N	GLY			48.953	9.002	0.644	1.00 1		Α
	MOTA	731	CA	GLY	Α	158	47.684	8.299	0.572	1.00 1	6.13	Α
	MOTA	732	C	GLY	Α	158	47.000	8.383	1.920	1.00 1	4.94	Α
	ATOM	733	0	GLY	Α	158	47.445	7.756	2.879	1.00 1	6.28	Α
55	ATOM	734	N	LEU	Α	159	45.915	9.145	1.989	1.00 1	3.50	Α
	MOTA	735	CA	LEU	Α	159	45.191	9.340	3.241	1.00 1	5.20	Α
	MOTA	736	CB	LEU	Α	159	45.031	10.835	3.517	1.00 1		Α
	ATOM	737	CG	LEU			46.270	11.726	3.385	1.00 1		Α
	ATOM	738	CD1	LEU			45.847	13.188	3.477	1.00 1		А

	MOTA	739	CD2	LEU	А	159	47.275	11.390	4.471	1.00 1	4.71	A
	ATOM	740	C			159	43.809	8.716	3.232	1.00 1		A
	ATOM	741	o			159	43.232	8.472	2.177	1.00 1		A
	ATOM	742	N	SER			43.268	8.469	4.418	1.00 1		A
5	ATOM	743	CA	SER			41.932	7.917	4.498	1.00 1		A
	ATOM	744	CB	SER			41.566	7.582	5.949	1.00 2		A
	ATOM	745	OG	SER			41.901	8.629	6.833	1.00 2		A
	ATOM	746	C	SER			40.987	8.968	3.924	1.00 2		A
1.0	ATOM	747	0	SER			41.213	10.173	4.062	1.00 1		A
10	MOTA	748	N	TYR			39.945	8.508	3.250	1.00 1		A
	MOTA	749	CA	TYR			38.975	9.406	2.644	1.00 2		A
	MOTA	750	CB	TYR			38.471	8.785	1.332	1.00 2		A
	MOTA	751	CG	TYR			37.314	9.502	0.666	1.00 2		A
	ATOM	752		TYR			37.222	10.895	0.682	1.00 1		A
15	MOTA	753	CE1				36.180	11.557	0.029	1.00 2		A
	ATOM	754	CD2				36.333	8.784	-0.020	1.00 2		A
	ATOM	755	CE2	TYR	Α	161	35.287	9.436	-0.678	1.00 2		A
	MOTA	756	CZ	TYR	Α	161	35.218	10.822	-0.648	1.00 2	2.32	A
	MOTA	757	OH	TYR	Α	161	34.194	11.471	-1.298	1.00 2	3.03	A
20	ATOM	758	C	TYR	Α	161	37.812	9.681	3.598	1.00 2	0.14	A
	ATOM	759	0	TYR	Α	161	36.959	8.819	3.810	1.00 1	9.53	A
	ATOM	760	N	ALA	А	162	37.791	10.880	4.178	1.00 1	9.92	A
	ATOM	761	CA	ALA	Α	162	36.721	11.271	5.099	1.00 2	1.07	A
	ATOM	762	CB	ALA			37.187	12.419	6.002	1.00 1		A
25	ATOM	763	C	ALA			35.542	11.712	4.238	1.00 2		A
	ATOM	764	ō	ALA			35.436	12.875	3.860	1.00 2		A
	ATOM	765	N	LYS			34.653	10.769	3.945	1.00 2		A
	ATOM	766	CA	LYS			33.503	11.017	3.080	1.00 2		A
	ATOM	767	CB	LYS			32.663	9.741	2.963	1.00 2		A
30	ATOM	768	CG	LYS			33.455	8.524	2.515	1.00 3		A
50	ATOM	769	CD	LYS			32.556	7.310	2.321	1.00 4		A
	ATOM	770	CE	LYS			33.373	6.034	2.321	1.00 4		A
	ATOM	771	NZ	LYS						1.00 4		A A
							34.143	5.735	3.430			
2.5	ATOM	772	С	LYS			32.581	12.186	3.411	1.00 2		A
35	ATOM	773	0	LYS			32.103	12.863	2.506	1.00 2		A
	ATOM	774	N	ASN			32.327	12.441	4.689	1.00 2		A
	MOTA	775	CA	ASN			31.420	13.522	5.033	1.00 2		A
	MOTA	776	CB	ASN			30.610	13.129	6.265	1.00 2		A
	MOTA	777	CG	ASN			29.537	12.101	5.932	1.00 2		A
40	MOTA	778		ASN			28.772	12.281	4.983	1.00 2		A
	ATOM	779		ASN			29.475	11.024	6.704	1.00 2		A
	ATOM	780	C	ASN			31.999	14.931	5.169	1.00 2		A
	MOTA	781	0	ASN	Α	164	31.306	15.856	5.589	1.00 2	3.98	A
	MOTA	782	N	GLY	Α	165	33.262	15.097	4.795	1.00 2	1.56	A
45	ATOM	783	CA	GLY	Α	165	33.873	16.414	4.836	1.00 2	4.39	A
	ATOM	784	C	GLY	Α	165	34.191	17.043	6.181	1.00 2	3.62	A
	ATOM	785	0	GLY	Α	165	34.380	16.352	7.177	1.00 2	3.26	A
	ATOM	786	N	GLU	Α	166	34.234	18.373	6.186	1.00 2	3.22	A
	ATOM	787	CA	GLU			34.563	19.176	7.362	1.00 2	4.54	A
50	MOTA	788	CB	GLU			35.055	20.558	6.913	1.00 2		A
	MOTA	789	CG	GLU			36.419	20.569	6.229	1.00 2		A
	ATOM	790	CD	GLU			36.699	21.889	5.517	1.00 3		A
	ATOM	791		GLU			36.081	22.906	5.889	1.00 2		A
	ATOM	792		GLU			37.544	21.916	4.596	1.00 2		A
55	ATOM	793	C	GLU			33.436	19.372	8.369	1.00 2		A
22	ATOM	794	0	GLU			32.279	19.541	8.001	1.00 2		A
	ATOM	795	N	LEU			33.791	19.341	9.649	1.00 2		A
	ATOM	795	CA.	LEU			32.813	19.370	10.707	1.00 2		A A
	MOTA	797	CB	LEU	А	тю/	33.497	19.481	12.073	1.00 2	2.32	A

	ATOM	798	CG	LEU	Α	167	32.706	19.923	13.306	1.00	22.04	A
	ATOM	799		LEU			31.454	19.074	13.463	1.00		A
	ATOM	800		LEU			33.597	19.805	14.537	1.00		A
	ATOM	801	C			167	32.193	20.971	10.529	1.00		A
5	ATOM	802	ō			167	31.047	21.209	10.907	1.00		A
	ATOM	803	N			168	32.960	21.887	9.948	1.00		A
	ATOM	804	CA	LEU			32.473	23.245	9.722	1.00		A
	ATOM	805	CB			168	33.560	24.099	9.066	1.00		A
	ATOM	806	CG			168	33.198	25.546	8.707	1.00		A
10									9.946			
10	ATOM	807		LEU			32.718	26.296		1.00		A
	MOTA	808		LEU			34.418	26.238	8.119	1.00		A
	MOTA	809	C			168	31.234	23.218	8.829	1.00		A
	MOTA	810	0			168	30.297	23.989	9.030	1.00		A
	ATOM	811	N			169	31.233	22.320	7.848	1.00		A
15	MOTA	812	CA			169	30.106	22.210	6.934	1.00		A
	MOTA	813	CB			169	30.324	21.064	5.945	1.00		A
	MOTA	814	CG			169	29.151	20.854	4.993	1.00		A
	MOTA	815	CD			169	29.407	19.728	3.998	1.00		A
	MOTA	816	CE	LYS			29.462	18.372	4.683	1.00		A
20	MOTA	817	NZ			169	29.622	17.263	3.702	1.00		A
	MOTA	818	C	LYS	Α	169	28.801	21.985	7.682	1.00	28.12	A
	MOTA	819	0	LYS	Α	169	27.785	22.608	7.371	1.00	28.08	A
	ATOM	820	N	TYR	Α	170	28.826	21.094	8.668	1.00	26.53	A
	MOTA	821	CA	TYR	Α	170	27.624	20.791	9.434	1.00	26.95	A
25	ATOM	822	CB	TYR	Α	170	27.810	19.476	10.193	1.00	25.03	A
	ATOM	823	CG	TYR	Α	170	27.898	18.300	9.251	1.00	26.65	A
	ATOM	824	CD1	TYR	Α	170	26.745	17.661	8.790	1.00	28.27	A
	ATOM	825	CE1	TYR	Α	170	26.814	16.642	7.839	1.00	26.85	A
	ATOM	826		TYR			29.127	17.884	8.742	1.00		A
30	ATOM	827	CE2	TYR			29.209	16.869	7.792	1.00		A
	ATOM	828	CZ			170	28.049	16.254	7.343	1.00		A
	ATOM	829	OH			170	28.130	15.268	6.382	1.00		A
	ATOM	830	С			170	27.229	21.918	10.376	1.00		A
	ATOM	831	ō			170	26.045	22.122	10.642	1.00		A
35	ATOM	832	N			171	28.208	22.660	10.882	1.00		A
55	ATOM	833	CA			171	27.883	23.770	11.763	1.00		A
	ATOM	834	CB			171	29.151	24.435	12.337	1.00		A
	ATOM	835		ILE			28.773	25.705	13.084	1.00		A
	ATOM	836		ILE			29.872	23.458	13.272	1.00		A
40	ATOM	837		ILE			31.163	23.996	13.856	1.00		A
40	ATOM	838	C			171	27.094	24.796	10.944	1.00		A
	ATOM	839	o			171	26.088	25.335	11.407	1.00		A
	ATOM	840	N	ARG			27.546	25.047	9.719	1.00		A
										1.00		
45	ATOM	841	CA	ARG			26.874	26.000	8.844			A
43	ATOM	842	CB	ARG			27.734	26.314	7.616	1.00		A
	ATOM	843	CG	ARG			29.057	27.011	7.912	1.00		A
	MOTA	844	CD	ARG			29.708	27.492	6.616	1.00		A
	MOTA	845	NE	ARG			31.037	28.070	6.812	1.00		A
	MOTA	846	CZ	ARG			31.314	29.059	7.658	1.00		A
50	MOTA	847		ARG			30.355	29.593	8.406	1.00		A
	MOTA	848		ARG			32.553	29.526	7.748	1.00		A
	MOTA	849	C	ARG			25.528	25.459	8.378	1.00		A
	MOTA	850	0	ARG			24.550	26.200	8.288	1.00		A
	MOTA	851	N	LYS			25.481	24.163	8.092	1.00		A
55	MOTA	852	CA	LYS			24.259	23.528	7.619	1.00		A
	ATOM	853	CB			173	24.523	22.061	7.272	1.00		A
	MOTA	854	CG			173	23.279	21.298	6.830	1.00		A
	MOTA	855	CD			173	23.557	19.808	6.653	1.00		A
	MOTA	856	CE	LYS	Α	173	24.477	19.530	5.469	1.00	52.63	A

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	857 858 859 860 861 862 863	NZ C O N CA	LYS LYS LYS ILE	A A	173	23.855 23.089 21.981	19.894 23.608 23.960	4.160 8.595 8.201	1.00 54.61 1.00 39.30 1.00 39.62	A A A
	ATOM ATOM ATOM ATOM ATOM ATOM	859 860 861 862	O N	LYS	Α						
	ATOM ATOM ATOM ATOM ATOM ATOM	859 860 861 862	O N	LYS	Α						
	ATOM ATOM ATOM ATOM ATOM	860 861 862	N								
	ATOM ATOM ATOM ATOM	861 862				174	23.320	23.282	9.863	1.00 37.96	A
	ATOM MOTA MOTA	862	CA.	ILE			22.229	23.314	10.833	1.00 37.36	A
10	MOTA MOTA		CB	ILE			22.159	21.998	11.652	1.00 37.44	A
10	ATOM			ILE			22.159	20.802	10.709	1.00 37.44	A
10											
10		864		ILE			23.397	21.850	12.532	1.00 37.25	A
10	MOTA	865		ILE			23.355	20.620	13.418	1.00 36.85	A
	MOTA	866	C	ILE			22.259	24.492	11.801	1.00 36.71	A
	ATOM	867	0	ILE			21.448	24.556	12.724	1.00 38.05	A
	ATOM	868	N	GLY			23.185	25.423	11.592	1.00 35.48	A
	MOTA	869	CA	GLY	Α	175	23.265	26.585	12.462	1.00 35.29	A.
	MOTA	870	C	GLY	Α	175	24.053	26.360	13.737	1.00 35.06	A
15	MOTA	871	0	GLY	Α	175	25.066	27.019	13.970	1.00 37.46	A
	ATOM	872	N	SER	Α	176	23.581	25.441	14.571	1.00 33.94	A
	MOTA	873	CA	SER	Α	176	24.253	25.113	15.822	1.00 32.84	A
	ATOM	874	CB	SER	Α	176	23.938	26.155	16.901	1.00 33.54	A
	ATOM	875	OG	SER	Α	176	22.599	26.056	17.347	1.00 34.86	A
20	ATOM	876	C	SER			23.796	23.731	16.276	1.00 32.34	A
	ATOM	877	ō	SER			22.726	23.263	15.884	1.00 32.82	A
	ATOM	878	N	PHE			24.609	23.085	17.103	1.00 29.39	A
	ATOM	879	CA	PHE			24.313	21.743	17.597	1.00 27.20	A
	ATOM	880	CB	PHE			25.621	20.989	17.865	1.00 26.39	A
25	ATOM	881	CG	PHE			26.372	20.585	16.622	1.00 26.39	A
23											
	ATOM	882		PHE			26.210	21.277	15.426	1.00 25.30	A
	MOTA	883		PHE			27.266	19.516	16.662	1.00 26.05	A
	MOTA	884		PHE			26.923	20.912	14.290	1.00 26.59	A
	MOTA	885		PHE			27.986	19.143	15.532	1.00 26.06	A
30	MOTA	886	CZ	PHE			27.815	19.841	14.343	1.00 25.42	A
	ATOM	887	C	PHE			23.500	21.752	18.884	1.00 27.00	A
	ATOM	888	0	PHE			23.704	22.610	19.747	1.00 26.48	A
	MOTA	889	N	ASP	Α	178	22.578	20.802	19.022	1.00 26.70	A
	MOTA	890	CA	ASP	Α	178	21.816	20.729	20.260	1.00 26.35	A
35	ATOM	891	CB	ASP	Α	178	20.621	19.773	20.142	1.00 29.90	A
	ATOM	892	CG	ASP	Α	178	21.020	18.372	19.720	1.00 32.28	A
	ATOM	893	OD1	ASP	Α	178	22.157	17.949	20.014	1.00 35.21	A
	MOTA	894	OD2	ASP	А	178	20.179	17.683	19.105	1.00 34.79	A
	MOTA	895	C	ASP			22.810	20.228	21.311	1.00 25.03	A
40	MOTA	896	0	ASP			23.974	19.968	20.992	1.00 21.24	A
	ATOM	897	N	GLU			22.361	20.083	22.552	1.00 23.60	A
	ATOM	898	CA	GLU			23.247	19.644	23.619	1.00 25.18	A
	ATOM	899	CB	GLU			22.542	19.770	24.971	1.00 27.60	A
	ATOM	900	CG	GLU			23.324	19.176	26.130	1.00 32.58	A
45	ATOM	901	CD	GLU						1.00 35.82	A
43							22.997	19.845	27.449		
	ATOM	902		GLU			21.825	20.224	27.645	1.00 35.95	A
	MOTA	903		GLU			23.912	19.984	28.291	1.00 38.19	A
	MOTA	904	С	GLU			23.808	18.235	23.450	1.00 24.08	A
	MOTA	905	0	GLU			24.977	17.989	23.756	1.00 22.79	A
50	MOTA	906	N	THR			22.983	17.316	22.961	1.00 23.36	A
	MOTA	907	CA	THR			23.412	15.935	22.761	1.00 22.15	A
	MOTA	908	CB	THR			22.224	15.054	22.320	1.00 23.77	A
	MOTA	909		THR			21.222	15.075	23.341	1.00 26.37	A
	MOTA	910		THR			22.670	13.616	22.088	1.00 22.66	A
55	MOTA	911	C	THR	Α	180	24.533	15.830	21.724	1.00 22.01	A
	ATOM	912	0	THR	Α	180	25.533	15.141	21.944	1.00 19.87	A
	ATOM	913	N	CYS			24.365	16.511	20.596	1.00 21.21	A
	ATOM	914	CA	CYS			25.372	16.480	19.541	1.00 22.22	A
	ATOM	915	CB	CYS	А	181	24.800	17.065	18.250	1.00 24.62	A

	MOTA	916	SG	CYS	А	181	23.435	16.080	17.560	1.00 29.50	A
	ATOM	917	C	CYS			26.633	17.232	19.954	1.00 23.07	A
	ATOM	918	o	CYS			27.746	16.827	19.608	1.00 23.95	A
	ATOM	919	N	THR			26.463	18.325	20.695	1.00 23.33	A
5	ATOM	920	CA	THR			27.606	19.103	21.161	1.00 22.76	A
,											
	MOTA	921	CB	THR			27.167	20.346	21.978	1.00 21.37	A
	ATOM	922		THR			26.459	21.262	21.134	1.00 22.50	A
	MOTA	923		THR			28.379	21.046	22.565	1.00 18.36	A
	MOTA	924	С	THR			28.454	18.215	22.071	1.00 21.48	A
10	MOTA	925	0	THR			29.669	18.090	21.894	1.00 19.95	A
	MOTA	926	N	ARG			27.798	17.602	23.050	1.00 18.97	A
	MOTA	927	CA	ARG			28.468	16.723	23.996	1.00 19.39	A
	MOTA	928	CB	ARG			27.455	16.140	24.984	1.00 19.46	A
	MOTA	929	CG	ARG			28.030	15.062	25.887	1.00 18.77	A
15	MOTA	930	CD	ARG			27.021	14.571	26.925	1.00 21.19	A
	MOTA	931	NE	ARG	Α	183	26.605	15.642	27.824	1.00 19.46	A
	MOTA	932	CZ	ARG	Α	183	25.496	16.362	27.679	1.00 20.45	A
	MOTA	933	NH1	ARG	Α	183	24.672	16.123	26.666	1.00 19.81	A
	MOTA	934	NH2	ARG	Α	183	25.224	17.338	28.539	1.00 17.11	A
20	MOTA	935	C	ARG	Α	183	29.206	15.577	23.302	1.00 20.02	A
	MOTA	936	0	ARG	Α	183	30.383	15.333	23.573	1.00 19.97	A
	MOTA	937	N	PHE	Α	184	28.520	14.871	22.409	1.00 19.24	A
	MOTA	938	CA	PHE			29.144	13.746	21.722	1.00 18.04	A
	MOTA	939	CB	PHE			28.158	13.078	20.764	1.00 21.05	A
25	ATOM	940	CG	PHE			28.719	11.857	20.098	1.00 22.67	A
	ATOM	941		PHE			28.717	10.630	20.754	1.00 22.97	A
	ATOM	942	CD2	PHE			29.317	11.949	18.850	1.00 19.97	A
	ATOM	943	CE1	PHE			29.308	9.510	20.176	1.00 23.53	A
	ATOM	944	CE2	PHE			29.915	10.833	18.263	1.00 24.11	A
30	ATOM	945	CZ	PHE			29.910	9.613	18.928	1.00 22.97	A
30	ATOM	945	C	PHE			30.403	14.127	20.941	1.00 22.97	A
		947								1.00 17.99	
	ATOM		0	PHE			31.461	13.531	21.130		A
	MOTA	948	N	TYR			30.292	15.110	20.056	1.00 15.73	A
2.5	MOTA	949	CA	TYR			31.443	15.519	19.265	1.00 15.72	A
35	MOTA	950	CB	TYR			30.992	16.413	18.111	1.00 17.33	A
	MOTA	951	CG	TYR			30.364	15.584	17.015	1.00 19.37	A
	MOTA	952		TYR			31.159	14.809	16.168	1.00 16.53	A
	MOTA	953		TYR			30.590	13.952	15.232	1.00 18.12	A
	MOTA	954		TYR			28.976	15.484	16.892	1.00 18.18	A
40	MOTA	955		TYR			28.398	14.623	15.956	1.00 18.90	A
	MOTA	956	CZ	TYR			29.211	13.861	15.133	1.00 18.41	A
	MOTA	957	OH	TYR			28.650	12.995	14.218	1.00 20.48	A
	MOTA	958	C	TYR			32.544	16.172	20.083	1.00 15.79	A
	MOTA	959	0	TYR			33.720	16.015	19.766	1.00 17.69	A
45	MOTA	960	N	THR	Α	186	32.176	16.887	21.142	1.00 15.68	A
	MOTA	961	CA	THR	Α	186	33.184	17.504	21.997	1.00 16.03	A
	MOTA	962	CB	THR	Α	186	32.559	18.403	23.094	1.00 16.62	A
	MOTA	963	OG1	THR	Α	186	31.866	19.503	22.481	1.00 14.79	A
	MOTA	964	CG2	THR	Α	186	33.656	18.953	24.019	1.00 14.68	A
50	MOTA	965	C	THR	Α	186	33.954	16.375	22.680	1.00 15.59	A
	MOTA	966	0	THR	Α	186	35.176	16.443	22.823	1.00 13.77	A
	MOTA	967	N	ALA	А	187	33.234	15.333	23.097	1.00 14.06	A
	ATOM	968	CA	ALA			33.869	14.196	23.757	1.00 14.74	A
	ATOM	969	CB	ALA			32.810	13.195	24.224	1.00 14.32	A
55	ATOM	970	C	ALA			34.875	13.509	22.821	1.00 14.41	A
	ATOM	971	0	ALA			35.972	13.136	23.247	1.00 15.61	A
	ATOM	972	N	GLU			34.516	13.340	21.549	1.00 14.01	A
	ATOM	973	CA	GLU			35.443	12.704	20.615	1.00 14.01	A
	ATOM	974	CB	GLU			34.782	12.449	19.251	1.00 13.30	A
	111 011	2/1	CD	CHO	**	100	51.702	12.443	10.201	1.00 12.00	- A

	3.0001	0.25	00	OT 11	-	100	22 600	11 454	10 000	1 00	10 71	
	ATOM	975	CG	GLU			33.622	11.454	19.282		12.71	A
	MOTA	976	CD	GLU			33.464	10.685	17.979		15.01	A
	ATOM	977	OE1	GLU	Α	188	33.687	11.275	16.899	1.00	13.21	A
	ATOM	978	OE2	GLU	Α	188	33.110	9.484	18.031	1.00	17.69	A
5	ATOM	979	C	GLU	А	188	36.682	13.582	20.436	1.00	13.34	A
	MOTA	980	ō	GLU			37.803	13.085	20.408		14.69	A
	ATOM	981	N	ILE			36.486	14.893	20.326		13.52	A
									20.326		13.35	A
	MOTA	982	CA	ILE			37.627	15.787				
	MOTA	983	CB	ILE			37.169	17.247	19.939		13.95	A
10	MOTA	984		ILE			38.381	18.165	19.822		12.47	A
	MOTA	985	CG1	ILE	Α	189	36.302	17.332	18.671	1.00	13.44	A
	ATOM	986	CD1	ILE	Α	189	35.588	18.664	18.491	1.00	14.29	A
	ATOM	987	С	ILE	Α	189	38.530	15.702	21.394	1.00	14.63	A
	ATOM	988	0	ILE	Α	189	39.753	15.595	21.271	1.00	12.97	A
15	ATOM	989	N	VAL			37.927	15.751	22.582		14.35	A
	ATOM	990	CA	VAL			38.684	15.655	23.832		13.22	A
	ATOM	991	CB	VAL			37.743	15.690	25.061		14.28	A
				VAL			38.509	15.267	26.326		15.08	
	MOTA	992										A
	MOTA	993		VAL			37.160	17.082	25.233		12.08	A
20	MOTA	994	C	VAL			39.468	14.338	23.859		14.61	A
	MOTA	995	0	VAL			40.634	14.304	24.250		13.72	A
	MOTA	996	N	SER	Α	191	38.825	13.254	23.432	1.00	15.26	A
	ATOM	997	CA	SER	Α	191	39.478	11.943	23.421	1.00	16.81	A
	ATOM	998	CB	SER	Α	191	38.470	10.857	23.041	1.00	16.14	A
25	ATOM	999	OG	SER	Α	191	39.018	9.569	23.238	1.00	16.94	A
	ATOM	1000	C	SER			40.649	11.928	22.441		16.58	A
	ATOM	1001	o	SER			41.697	11.335	22.713		13.96	A
	ATOM	1002	N	ALA			40.468	12.586	21.300		15.26	A
	ATOM	1003	CA	ALA			41.518	12.645	20.292		14.37	A
30												
30	MOTA	1004	CB	ALA			40.989	13.296	19.016		14.43	A
	MOTA	1005	C	ALA			42.695	13.440	20.845		16.46	A
	MOTA	1006	0	ALA			43.851	13.038	20.697		17.96	A
	MOTA	1007	N	LEU			42.401	14.563	21.496		15.02	A
	MOTA	1008	CA	LEU	Α	193	43.459	15.392	22.067	1.00	15.42	A
35	ATOM	1009	CB	LEU	Α	193	42.884	16.712	22.600	1.00	12.88	A
	ATOM	1010	CG	LEU	Α	193	42.445	17.721	21.525	1.00	15.97	A
	MOTA	1011	CD1	LEU			41.869	18.979	22.190	1.00	13.97	A
	MOTA	1012		LEU			43.642	18.088	20.655	1.00	14.58	A
	ATOM	1013	c	LEU			44.211	14.659	23.174		14.49	A
40	ATOM	1014	o	LEU			45.427	14.813	23.310		16.56	A
40	ATOM	1015	N	GLU			43.500	13.870	23.975		13.96	A
	ATOM	1016	CA	GLU			44.179	13.123	25.032		14.08	A
	MOTA	1017	CB	GLU			43.190	12.295	25.857		14.65	A
	MOTA	1018	CG	GLU			43.882	11.301	26.789		17.09	A
45	MOTA	1019	CD	GLU			42.924	10.592	27.730		19.59	A
	MOTA	1020		GLU			41.809	10.237	27.295	1.00	19.25	A
	MOTA	1021	OE2	GLU	Α	194	43.302	10.380	28.906	1.00	20.20	A
	ATOM	1022	C	GLU	Α	194	45.208	12.199	24.386	1.00	13.57	A
	ATOM	1023	0	GLU	Α	194	46.337	12.093	24.847	1.00	14.23	A
50	MOTA	1024	N	TYR	Α	195	44.822	11.544	23.301	1.00	14.89	A
	MOTA	1025	CA	TYR			45.743	10.642	22.618		16.58	A
	ATOM	1026	CB	TYR			45.030	9.910	21.488		17.29	A
	ATOM	1027	CG	TYR			45.956	9.058	20.649		17.92	A
	MOTA	1028		TYR			46.347	7.788	21.077		17.96	A
55	MOTA	1029		TYR			47.203	6.996	20.304		19.77	A
	MOTA	1030	CD2				46.445	9.524	19.428		16.67	A
	MOTA	1031		TYR			47.299	8.744	18.650		18.51	A
	MOTA	1032	CZ	TYR	Α	195	47.671	7.481	19.094	1.00	20.24	A
	MOTA	1033	OH	TYR	Α	195	48.506	6.705	18.325	1.00	21.89	A

			_		_						
	ATOM	1034	C	TYR			46.917	11.419	22.035	1.00 16.9	
	ATOM	1035	0	TYR	А	195	48.081	11.047	22.203	1.00 14.6	1 A
	ATOM	1036	N	LEU	n	106	46.599	12,507	21.347	1.00 16.3	0 A
	MOTA	1037	CA	LEU	Α	196	47.619	13.328	20.720	1.00 18.1	
5	ATOM	1038	CB	LEU	А	196	46.969	14.502	19.982	1.00 18.5	9 A
	ATOM	1039	CG	LEU	Z.	196	47.834	15.203	18.935	1.00 22.5	1 A
	MOTA	1040		LEU			48.222	14.206	17.841	1.00 20.9	
	ATOM	1041	CD2	LEU	Α	196	47.060	16.375	18.338	1.00 22.9	8 A
	ATOM	1042	C	LEU	A	196	48.592	13.844	21.763	1.00 17.7	5 A
10	ATOM	1043	0	LEU			49.801	13.644	21.649	1.00 18.3	
10											
	MOTA	1044	N	HIS			48.064	14.495	22.792	1.00 17.1	
	ATOM	1045	CA	HIS	Α	197	48.913	15.042	23.842	1.00 18.4	7 A
	ATOM	1046	CB	HIS	A	197	48.069	15.866	24.817	1.00 15.9	0 A
	ATOM	1047	CG	HIS			47.571	17.152	24.231	1.00 19.1	
15	MOTA	1048		HIS			47.830	17.745	23.038	1.00 18.2	
	ATOM	1049	ND1	HIS	Α	197	46.704	17.992	24.897	1.00 17.4	7 A
	ATOM	1050	CE1	HIS	А	197	46.450	19.047	24.139	1.00 19.7	4 A
	ATOM	1051		HIS			47.119	18.921	23.007	1.00 15.6	
	MOTA	1052	С	HIS	А	197	49.696	13.958	24.572	1.00 19.4	0 A
20	ATOM	1053	0	HIS	Α	197	50.823	14.192	25.021	1.00 19.4	2 A
	ATOM	1054	N	GLY	Δ	198	49.106	12.770	24.679	1.00 18.5	9 A
	MOTA	1055	CA	GLY			49.793	11.675	25.339	1.00 19.6	
	MOTA	1056	С	GLY	Α	198	51.075	11.307	24.612	1.00 21.8	6 A
	ATOM	1057	0	GLY	Α	198	51.963	10.682	25.186	1.00 23.0	9 A
25	ATOM	1058	N	LYS	Δ	199	51.174	11.687	23.341	1.00 22.8	1 A
23											
	MOTA	1059	CA	LYS			52.368	11.401	22.549	1.00 24.4	
	ATOM	1060	CB	LYS	Α	199	51.990	10.905	21.154	1.00 26.0	0 A
	ATOM	1061	CG	LYS	Α	199	51.378	9.520	21.133	1.00 30.9	8 A
	ATOM	1062	CD	LYS			51.291	9.002	19.708	1.00 36.8	
30											
30	MOTA	1063	CE	LYS			50.832	7.559	19.682	1.00 40.3	
	ATOM	1064	NZ	LYS	Α	199	51.646	6.691	20.581	1.00 43.4	8 A
	MOTA	1065	C	LYS	А	199	53.253	12.631	22.414	1.00 23.8	8 A
	ATOM	1066	ō	LYS			54.144	12.669	21.568	1.00 24.9	
	MOTA	1067	N	GLY			52.997	13.638	23.243	1.00 24.0	
35	MOTA	1068	CA	GLY	Α	200	53.790	14.853	23.203	1.00 22.1	2 A
	ATOM	1069	C	GLY	А	200	53.665	15.632	21.907	1.00 22.1	4 A
	ATOM	1070	o	GLY			54.632	16.231	21.439	1.00 22.4	
	MOTA	1071	N	ILE			52.475	15.630	21.320	1.00 20.0	
	MOTA	1072	CA	ILE	Α	201	52.252	16.355	20.080	1.00 18.9	3 A
40	MOTA	1073	CB	ILE	Α	201	51.784	15.414	18.955	1.00 19.7	0 A
	ATOM	1074	cco	ILE			51.414	16.226	17.716	1.00 20.1	
	MOTA	1075		ILE			52.880	14.395	18.636	1.00 20.0	
	ATOM	1076	CD1	ILE	Α	201	52.408	13.258	17.745	1.00 22.7	5 A
	ATOM	1077	C	ILE	А	201	51.193	17.425	20.270	1.00 19.8	7 A
45	ATOM	1078	0	ILE			50.121	17.161	20.817	1.00 20.0	
75											
	MOTA	1079	N	ILE			51.508	18.633	19.815	1.00 19.9	
	ATOM	1080	CA	ILE	Α	202	50.601	19.772	19.891	1.00 20.4	5 A
	MOTA	1081	CB	ILE	A	202	51.352	21.040	20.356	1.00 22.2	1 A
	ATOM	1082		ILE			50.381	22.220	20.470	1.00 22.6	
50	MOTA	1083		ILE			52.033	20.775	21.700	1.00 24.1	
	MOTA	1084	CD1	ILE	Α	202	52.914	21.920	22.169	1.00 25.3	9 A
	MOTA	1085	C	ILE	A	202	50.105	19.999	18.464	1.00 20.7	1 A
			o	ILE			50.910	20.067	17.538	1.00 19.4	
	MOTA	1086									
	MOTA	1087	N	HIS	Α	203	48.795	20.108	18.270	1.00 18.6	5 A
55	ATOM	1088	CA	HIS	Α	203	48.280	20.319	16.919	1.00 18.0	2 A
	ATOM	1089	CB	HIS			46.775	20.057	16.874	1.00 16.3	
	MOTA	1090	CG	HIS			46.199	20.136	15.495	1.00 18.3	
	ATOM	1091		HIS			46.043	21.186	14.655	1.00 16.4	
	ATOM	1092	ND1	HIS	Α	203	45.759	19.026	14.806	1.00 19.5	0 A

	ATOM	1093	CE1	HIS	Δ	203	45.359	19.389	13.600	1.00	17.64	A
	ATOM	1094		HIS			45.522	20.694	13.483		20.87	A
	ATOM	1095	C	HIS			48.589	21.738	16.405		18.92	A
-	MOTA	1096	0	HIS			49.073	21.906	15.282		16.21	A
5	MOTA	1097	N	ARG			48.301	22.744	17.232		18.60	A
	MOTA	1098	CA	ARG			48.552	24.157	16.914		19.81	A
	ATOM	1099	CB	ARG			49.998	24.365	16.458		21.61	A
	MOTA	1100	CG	ARG			51.024	24.137	17.550		23.82	A
	MOTA	1101	CD	ARG			52.323	24.870	17.252		27.62	A
10	MOTA	1102	NE	ARG			52.932	24.449	15.994		29.43	A.
	MOTA	1103	CZ	ARG	Α	204	54.125	24.861	15.572	1.00	33.10	A
	ATOM	1104	NH1	ARG	Α	204	54.835	25.706	16.311	1.00	32.12	A
	MOTA	1105	NH2	ARG	Α	204	54.614	24.426	14.418	1.00	30.25	A
	ATOM	1106	C	ARG	Α	204	47.624	24.830	15.905	1.00	20.03	A
15	ATOM	1107	0	ARG	Α	204	47.711	26.038	15.698	1.00	20.88	A
	ATOM	1108	N	ASP	А	205	46.755	24.071	15.255	1.00	18.96	A
	ATOM	1109	CA	ASP	А	205	45.828	24.692	14.325	1.00	17.90	A
	ATOM	1110	CB	ASP			46.418	24.741	12.914		18.95	A
	ATOM	1111	CG	ASP			45.655	25.688	12.008		20.36	A
20	ATOM	1112		ASP			44.939	26.560	12.545		20.35	A
20	ATOM	1113		ASP			45.772	25.573	10.771		22.49	A
	ATOM	1114	C	ASP			44.500	23.956	14.328		19.60	A
	ATOM	1115	0	ASP			43.876	23.751	13.287		21.53	A
25	MOTA	1116	N	LEU			44.063	23.569	15.521		18.53	A
23	ATOM	1117	CA				42.813	22.851	15.667		19.18	A
	MOTA	1118	CB	LEU			42.693	22.295	17.087		18.94	A
	ATOM	1119	CG	LEU			41.511	21.358	17.346		23.10	A
	MOTA	1120					41.615	20.142	16.436		23.01	A
	MOTA	1121		LEU			41.504	20.933	18.808		22.97	A
30	MOTA	1122	C	LEU			41.639	23.772	15.361		19.05	A
	MOTA	1123	0	LEU			41.556	24.880	15.886		19.25	A
	MOTA	1124	N	LYS			40.740	23.307	14.500		17.54	A
	MOTA	1125	CA	LYS			39.564	24.081	14.110		18.60	A
	MOTA	1126	CB	LYS	Α	207	39.980	25.248	13.196	1.00	18.98	A
35	ATOM	1127	CG	LYS	Α	207	40.786	24.817	11.982	1.00	18.20	A
	ATOM	1128	CD	LYS	Α	207	41.246	26.000	11.139	1.00	21.42	A
	MOTA	1129	CE	LYS	Α	207	42.223	25.537	10.062	1.00	23.21	A
	MOTA	1130	NZ	LYS	Α	207	42.561	26.604	9.084	1.00	29.61	A
	MOTA	1131	C	LYS	Α	207	38.566	23.181	13.388	1.00	18.18	A
40	MOTA	1132	0	LYS	Α	207	38.921	22.100	12.915	1.00	18.11	A
	ATOM	1133	N	PRO	А	208	37.298	23.614	13.293	1.00	20.26	A
	ATOM	1134	CD	PRO	А	208	36.713	24.833	13.882	1.00	18.79	A
	ATOM	1135	CA	PRO	А	208	36,272	22.814	12.616	1.00	19.67	A
	ATOM	1136	CB	PRO			35.063	23.742	12.608		19.45	A
45	ATOM	1137	CG	PRO			35.231	24.509	13.891		21.81	A
	ATOM	1138	C	PRO			36.674	22.372	11.209		21.04	A
	ATOM	1139	ŏ	PRO			36.264	21.307	10.751		21.19	A
	ATOM	1140	N	GLU			37.474	23.188	10.528		21.69	A
	ATOM	1141	CA	GLU			37.928	22.872	9.170		22.64	A
50	ATOM	1142	CB	GLU			38.644	24.084	8.558		23.65	A
50												
	MOTA	1143	CG	GLU			39.253	23.825	7.185		27.24	A
	MOTA	1144	CD	GLU			40.155	24.958	6.716		29.40	A
	MOTA	1145		GLU			39.660	26.094	6.553		29.68	A
	MOTA	1146		GLU			41.363	24.711	6.511		30.07	A
55	MOTA	1147	C	GLU			38.879	21.668	9.159		22.28	A
	MOTA	1148	0	GLU			38.955	20.933	8.170		21.36	A
	MOTA	1149	N	ASN			39.600	21.490	10.263		19.90	A
	MOTA	1150	CA	ASN			40.574	20.412	10.436		19.44	A
	MOTA	1151	CB	ASN	Α	210	41.744	20.912	11.287	1.00	20.07	A

	ATOM	1152	CG	ASN	Α	210	42.746	21.698	10.479	1.00	25.77	A
	ATOM	1153		ASN			43.571	22.427	11.029	1.00		A
	ATOM	1154		ASN			42.687	21.548	9.158	1.00		A
	ATOM	1155	C			210	40.005	19.151	11.078	1.00		A
5	ATOM	1156	Ö			210	40.712	18.154	11.234	1.00		A
,	ATOM	1157	N			211	38.739	19.202	11.469	1.00		A
	ATOM	1158	CA			211	38.090	18.058	12.085	1.00		A
	MOTA	1159	CB			211	37.336	18.488	13.354	1.00		A
	MOTA	1160		ILE			36.582	17.311	13.950	1.00		A
10	MOTA	1161		ILE			38.342	19.046	14.365	1.00		A
	MOTA	1162	CD1	ILE			37.720	19.669	15.590	1.00		A
	ATOM	1163	С			211	37.131	17.485	11.059	1.00		A
	MOTA	1164	0	ILE	Α	211	35.995	17.947	10.926	1.00	18.16	A
	ATOM	1165	N	LEU	Α	212	37.599	16.486	10.317	1.00	15.97	A
15	ATOM	1166	CA	LEU	Α	212	36.784	15.875	9.274	1.00	17.08	A
	ATOM	1167	CB	LEU	Α	212	37.685	15.249	8.202	1.00	17.78	A
	ATOM	1168	CG	LEU	А	212	38.785	16.157	7.640	1.00	18.92	A
	MOTA	1169	CD1	LEU	А	212	39.476	15.450	6.485	1.00	22.09	A
	ATOM	1170		LEU			38.188	17.482	7.166	1.00		A
20	ATOM	1171	C			212	35.843	14.825	9.837	1.00		A
20	ATOM	1172	ō			212	35.957	14.433	11.002	1.00		A
	ATOM	1173	N			213	34.915	14.368	9.000	1.00		A
	MOTA	1174	CA			213	33.942	13.362	9.403	1.00		A
	MOTA	1175	CB			213	32.556	14.004	9.487	1.00		A
25	MOTA	1176	CG			213	32.396	15.059	10.583	1.00		A
	MOTA	1177		LEU			31.124	15.837	10.367	1.00		A
	MOTA	1178		LEU			32.379	14.378	11.940	1.00		A
	MOTA	1179	С			213	33.914	12.187	8.426	1.00		A
	MOTA	1180	0	LEU	Α	213	33.743	12.379	7.218	1.00	19.55	A
30	MOTA	1181	N	ASN	Α	214	34.088	10.970	8.935	1.00	20.44	A
	ATOM	1182	CA	ASN	Α	214	34.055	9.814	8.049	1.00	23.77	A
	ATOM	1183	CB	ASN	Α	214	34.745	8.596	8.674	1.00	25.30	A
	ATOM	1184	CG	ASN	А	214	34.077	8,127	9.948	1.00	32.04	A
	ATOM	1185	OD1	ASN	А	214	32.908	8.422	10.206	1.00	34.43	A
35	ATOM	1186	ND2	ASN	А	214	34.818	7.369	10.752	1.00	33.85	A
	ATOM	1187	C			214	32.618	9.466	7.693	1.00		A
	ATOM	1188	o			214	31.672	10.113	8.150	1.00		A
	ATOM	1189	N			215	32.459	8.433	6.879	1.00		A
	ATOM	1190	CA			215	31.138	8.003	6.445	1.00		A
40	ATOM	1191	CB			215	31.275	6.796	5.513	1.00		A
40												
	ATOM	1192	CG			215	29.970	6.334	4.896	1.00		A
	MOTA	1193	CD			215	30.182	5.312	3.795	1.00		A
	MOTA	1194		GLU			30.817	4.268	4.065	1.00		A
	MOTA	1195		GLU			29.716	5.556	2.660	1.00		A
45	MOTA	1196	C			215	30.188	7.673	7.601	1.00		A
	MOTA	1197	0			215	28.971	7.769	7.447	1.00		A
	MOTA	1198	N	ASP	Α	216	30.737	7.287	8.752	1.00	26.77	A
	MOTA	1199	CA	ASP	Α	216	29.914	6.953	9.917	1.00	27.28	A
	ATOM	1200	CB	ASP	Α	216	30.538	5.795	10.696	1.00	31.27	A
50	MOTA	1201	CG	ASP	Α	216	30.390	4.466	9.979	1.00	37.61	A
	MOTA	1202	OD1	ASP	Α	216	29.274	4.170	9.499	1.00	39.45	A
	ATOM	1203		ASP			31.382	3.710	9.902	1.00		A
	ATOM	1204	c			216	29.697	8.135	10.862	1.00		A
	ATOM	1205	o			216	29.136	7.984	11.950	1.00		A
55	ATOM	1206	N			217	30.156	9.306	10.441	1.00		A
22	ATOM	1207	CA			217	30.136	10.527	11.218	1.00		
	ATOM	1207	CB			217				1.00		A A
							28.537	10.789	11.517			
	ATOM	1209	CG			217	27.742	11.186	10.274	1.00		A
	ATOM	1210	SD	MET	Α	217	28.464	12.616	9.430	1.00	27.57	A

	ATOM	1211	CE	MET	Α	217	27.6	679	13.974	10.3	32	1.00	26.68	A
	ATOM	1212	C			217	30.8		10.618	12.5			21.51	A
	ATOM	1213	0	MET			30.4		11.323	13.4			18.62	A
	ATOM	1214	N	HIS			31.9		9.892	12.5			20.10	A
5	ATOM	1215	CA	HIS			32.8		9.964	13.6			19.86	A
,	ATOM	1216	CB	HIS			33.4		8.594	13.9			20.21	A
	ATOM	1217	CG	HIS			32.5		7.667	14.6			22.40	A
		1217		HIS									21.27	
	MOTA						31.9		6.547	14.2				A
10	MOTA	1219		HIS			32.1		7.863	16.0			19.59	A
10	MOTA	1220		HIS			31.3		6.902	16.3			21.88	A
	MOTA	1221		HIS			31.1		6.091	15.3			22.08	A
	MOTA	1222	С	HIS			33.9		10.921	13.1			19.10	A
	MOTA	1223	0	HIS			34.1		11.004	11.9			20.31	A
	MOTA	1224	N			219	34.6		11.638	14.0			17.21	A
15	MOTA	1225	CA	ILE	Α	219	35.6	628	12.586	13.€	18	1.00	15.26	A
	MOTA	1226	CB	ILE	Α	219	35.9	987	13.614	14.7	16	1.00	15.38	A
	ATOM	1227	CG2	ILE	Α	219	34.	722	14.305	15.2	21	1.00	14.58	A
	MOTA	1228	CG1	ILE	Α	219	36.7	734	12.919	15.8	64	1.00	14.46	A
	ATOM	1229	CD1	ILE	Α	219	37.2	279	13.885	16.9	11	1.00	13.74	A
20	ATOM	1230	C	ILE	Α	219	36.9	929	11.944	13.1	61	1.00	16.21	A
	ATOM	1231	0	ILE	Α	219	37.2	238	10.799	13.5	0.0	1.00	15.88	A
	ATOM	1232	N	GLN	А	220	37.6	677	12.711	12.3	78	1.00	15.62	A
	ATOM	1233	CA			220	38.9		12.316	11.8			17.84	A
	ATOM	1234	CB			220	38.8		11.595	10.5			20.00	A
25	ATOM	1235	CG			220	38.4		10.129	10.6			26.97	A
	ATOM	1236	CD			220	38.6		9.343	9.3			29.95	A
	ATOM	1237		GLN			37.9		9.590	8.3			33.12	A
	ATOM	1237		GLN			39.5		8.393	9.3			30.47	A
	ATOM	1239	C			220	39.7		13.610	11.7			17.00	A
30			Ö			220				10.7				
30	ATOM	1240					39.6		14.339				18.27	A
	MOTA	1241	N			221	40.5		13.906	12.7			14.34	A
	ATOM	1242	CA			221	41.3		15.120	12.7			14.46	A
	MOTA	1243	CB			221	41.8		15.416	14.1			12.30	A
	MOTA	1244		ILE			42.7		16.656	14.1			14.78	A
35	MOTA	1245		ILE			40.6		15.613	15.1			13.92	A
	MOTA	1246		ILE			41.0		15.901	16.5			15.06	A
	ATOM	1247	С			221	42.5		14.996	11.7			15.44	A
	MOTA	1248	0			221	43.1		13.915	11.6			13.93	A
	MOTA	1249	N			222	42.8		16.101	11.1			15.36	A
40	MOTA	1250	CA	THR	Α	222	43.9	980	16.098	10.1	74	1.00	17.52	A
	MOTA	1251	CB	THR	Α	222	43.4	470	15.836	8.7	50	1.00	19.92	A
	ATOM	1252	OG1	THR	Α	222	44.5	587	15.637	7.8	75	1.00	18.78	A
	ATOM	1253	CG2	THR	Α	222	42.6	630	17.018	8.2	57	1.00	18.16	A
	ATOM	1254	С	THR	Α	222	44.7	735	17.428	10.1	92	1.00	19.60	A
45	ATOM	1255	0	THR	Α	222	44.5	509	18.257	11.0	84	1.00	18.59	A
	MOTA	1256	N	ASP			45.6		17.610	9.2			18.69	A
	ATOM	1257	CA	ASP			46.4		18.825	9.0			20.12	A
	ATOM	1258	CB	ASP			45.5		20.065	9.1			23.51	A
	ATOM	1259	CG	ASP			46.2		21.335	8.6			27.09	A
50	ATOM	1260		ASP			47.2		21.227	7.9			26.28	A
50	ATOM	1261		ASP			45.		22.438	9.0			26.15	A
	ATOM	1262	C	ASP			47.5		18.913	10.1			21.73	A
	ATOM	1263	o	ASP			47.4		19.751	11.0			22.76	A
	ATOM	1264	N			224	48.5		18.063	10.0			20.75	A
55	ATOM	1265	CA			224	49.6		17.988	11.0			20.11	A
	MOTA	1266	CB			224	49.8		16.527	11.4			20.62	A
	ATOM	1267	CG			224	48.6		15.991	12.2			21.41	A
	MOTA	1268		PHE			48.5		16.312	13.€			23.05	A
	ATOM	1269	CD2	PHE	Α	224	47.6	681	15.212	11.€	93	1.00	22.27	A

	ATOM	1270	CE1	PHE	А	224	47.528	15.868	14.389	1.00	23.30	A
	ATOM	1271	CE2	PHE	A	224	46.606	14.763	12.457	1.00	21.11	A
	MOTA	1272	CZ			224	46.530	15.093	13.807		22.02	A
	ATOM	1273	C	PHE	Α	224	50.957	18.583	10.619	1.00	20.45	A
5	ATOM	1274	0	PHE	Δ	224	51.905	18.547	11.407	1 00	20.73	A
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	ATOM	1275	N	GLY			51.049	19.125	9.412		22.02	A
	ATOM	1276	CA	GLY	Α	225	52.301	19.713	8.981	1.00	22.66	A
	ATOM	1277	С	GLY	75	225	52.742	20.822	9.920	1 00	24.99	A
	ATOM	1278	0	GLY			53.939	21.041	10.122		24.52	A
10	MOTA	1279	N	THR	Α	226	51.779	21.524	10.508	1.00	23.50	A
	ATOM	1280	CA	THR	75	226	52.106	22.613	11.416	1 00	25.16	A
	ATOM	1281	CB			226	51.199	23.829	11.160		24.76	A
	ATOM	1282	OG1	THR	Α	226	49.831	23.410	11.113	1.00	22.68	A
	ATOM	1283	CG2	THR	A	226	51.571	24.490	9.834	1.00	25.00	A
15	ATOM	1284	C			226	52.046	22.233	12.894		25.79	A
13												
	ATOM	1285	0	THR	А	226	52.019	23.100	13.768	1.00	24.54	A
	ATOM	1286	N	ALA	Α	227	52.037	20.935	13.173	1.00	24.97	A
	ATOM	1287	CA	ALA	75	227	52.004	20.475	14.550	1 00	25.49	A
	ATOM	1288	CB	ALA			51.659	18.993	14.607		22.85	A
20	ATOM	1289	C	ALA	Α	227	53.384	20.715	15.149	1.00	27.70	A
	ATOM	1290	0	ALA	Δ	227	54.331	21.047	14.435	1 00	26.60	A
	MOTA	1291	N	LYS			53.491	20.558	16.461		28.53	A
	ATOM	1292	CA	LYS	Α	228	54.760	20.745	17.149	1.00	32.12	A
	ATOM	1293	CB	LYS	A	228	54.699	21.974	18.054	1.00	33.81	A
25	ATOM	1294	CG	LYS			56.007	22.294	18.765		41.23	A
23												
	MOTA	1295	CD	LYS			57.082	22.725	17.768		47.57	A
	ATOM	1296	CE	LYS	Α	228	58.401	23.056	18.462	1.00	49.82	A
	ATOM	1297	NZ	LYS			59.459	23.425	17.480		51.49	A
	MOTA	1298	C	LYS			55.019	19.504	17.985		33.25	A
30	ATOM	1299	0	LYS	Α	228	54.190	19.129	18.815	1.00	33.70	A
	ATOM	1300	N	VAL	A	229	56.159	18.860	17.756	1.00	33.64	A.
	ATOM	1301	CA	VAL			56.516	17.661	18.501		34.66	A
	ATOM	1302	CB	VAL	A	229	57.248	16.646	17.609	1.00	33.50	A
	ATOM	1303	CG1	VAL	Α	229	57.619	15.419	18.415	1.00	32.34	A
35	MOTA	1304	cco	VAL	70	220	56.370	16.264	16.436		34.25	A
00												
	ATOM	1305	C			229	57.420	18.035	19.668		37.57	A
	ATOM	1306	0	VAL	Α	229	58.581	18.392	19.474	1.00	35.91	A
	ATOM	1307	N	LEU	Δ	230	56.877	17.948	20.878	1.00	40.57	A
	ATOM	1308	CA	LEU			57.615	18.289	22.088		46.10	A
40	ATOM	1309	CB	LEU	Α	230	56.654	18.417	23.270	1.00	44.71	A
	ATOM	1310	CG	LEU	А	230	55.627	19.545	23.207	1.00	44.50	A
	ATOM	1311		LEU			54.673	19,430	24.383		44.39	A
	ATOM	1312		LEU			56.340	20.885	23.214		44.81	A
	ATOM	1313	C	LEU	Α	230	58.695	17.279	22.440	1.00	50.42	A
45	ATOM	1314	0	LEU	Δ	230	58.603	16.104	22.089	1 00	51.64	A
	MOTA	1315	N			231	59.717	17.756	23.145		55.81	A
	ATOM	1316	CA	SER	Α	231	60.824	16.914	23.583	1.00	61.14	A
	ATOM	1317	CB	SER	A	231	62.077	17.200	22.750	1.00	61.27	A
	ATOM	1318	OG			231	62.444	18.568	22.823		62.85	A
50												
50	MOTA	1319	С	SER			61.124	17.126	25.071		64.65	A
	ATOM	1320	0	SER	Α	231	61.392	16.164	25.794	1.00	65.70	A
	ATOM	1321	N	PRO	A	232	61.081	18.387	25.549	1.00	67.54	A
											68.60	
	MOTA	1322	CD	PRO			60.854	19.651	24.823			A
	ATOM	1323	CA	PRO	Α	232	61.358	18.655	26.966	1.00	68.74	A
55	ATOM	1324	CB	PRO	Α	232	61.109	20.158	27.086	1.00	68.83	A
	ATOM	1325	CG			232	61.505	20.666	25.737		68.96	A
	MOTA	1326	C	PRO			60.460	17.846	27.899		69.17	A
	MOTA	1327	0	PRO	Α	232	59.335	17.494	27.541	1.00	69.94	A
	ATOM	1328	N	ALA	Α	237	57.424	23.198	27.637	1.00	80.06	A
												**

	ATOM	1329	CA	ALA .	Α	237	56.783	23.047	26.335	1.00	79.29	A
	ATOM	1330	CB	ALA .	А	237	55.275	22.907	26.512	1.00	78.64	A
	ATOM	1331	С	ALA .			57.092	24.239	25.433	1.00		A
	ATOM	1332	ō	ALA .			56.250	25.113	25.249	1.00		A
5	ATOM	1333	N	ALA .			58.297	24.280	24.871	1.00		A
-	ATOM	1334	CA	ALA .			58.683	25.383	23.992	1.00		A
	ATOM	1335	CB	ALA .			60.186	25.347	23.728	1.00		A
	ATOM	1336	C	ALA .			57.920	25.347	22.673	1.00		A
	ATOM	1337	0	ALA .			57.243	24.341	22.375	1.00		A
10												
10	ATOM	1338	N	ALA .			58.027	26.393	21.887	1.00		A
	MOTA	1339	CA	ALA .			57.338	26.452	20.603	1.00		A
	MOTA	1340	CB	ALA .			55.849	26.489	20.827	1.00		A
	MOTA	1341	C	ALA .			57.766	27.667	19.793	1.00		A
	MOTA	1342	0	ALA .			58.955	27.955	19.700	1.00		A
15	MOTA	1343	N	ASN .			56.781	28.357	19.214	1.00		A
	MOTA	1344	CA	ASN .			56.967	29.553	18.389	1.00		A
	MOTA	1345	CB	ASN .	A	240	58.151	30.400	18.874	1.00	71.47	A
	MOTA	1346	CG	ASN .	Α	240	59.459	30.055	18.174	1.00	72.06	A
	MOTA	1347	OD1	ASN .	A	240	59.575	30.149	16.943	1.00	72.03	A
20	ATOM	1348	ND2	ASN .	Α	240	60.470	29.665	18.964	1.00	71.91	A
	MOTA	1349	C	ASN .	A	240	57.188	29.178	16.928	1.00	69.41	A
	MOTA	1350	0	ASN .	Α	240	57.480	28.024	16.624	1.00	70.09	A
	ATOM	1351	N	ALA .	A	241	57.055	30.165	16.038	1.00	66.62	A
	ATOM	1352	CA	ALA .			57.246	30.013	14.585	1.00		A.
25	ATOM	1353	C	ALA .			55.952	30.080	13.772	1.00		A
	ATOM	1354	ō	ALA .			55.840	30.880	12.845	1.00		A
	ATOM	1355	СВ	ALA .			57.979	28.704	14.246	1.00		A
	ATOM	1356	N	PHE .			54.984	29.236	14.113	1.00		A
	ATOM	1357	CA	PHE .			53.712	29.196	13.394	1.00		A
30	ATOM	1358	CB	PHE .			53.419	27.767	12.923	1.00		A
30		1359	CG	PHE .			52.040	27.590	12.354	1.00		A
	ATOM			PHE .						1.00		
	ATOM	1360					51.731	28.067	11.085			A
	ATOM	1361		PHE .			51.038	26.975	13.102	1.00		A
2.5	MOTA	1362		PHE .			50.445	27.937	10.565	1.00		A
35	ATOM	1363		PHE .			49.751	26.840	12.594	1.00		A
	MOTA	1364	CZ	PHE .			49.453	27.323	11.322	1.00		A
	MOTA	1365	С	PHE .			52.534	29.688	14.229	1.00		A
	MOTA	1366	0	PHE .			52.502	29.505	15.444	1.00		A
	MOTA	1367	N	VAL .			51.566	30.305	13.557	1.00		A
40	MOTA	1368	CA	VAL .			50.355	30.809	14.200	1.00		A
	MOTA	1369	CB	VAL .			50.340	32.352	14.258	1.00		A
	MOTA	1370		VAL .			49.012	32.844	14.825	1.00		A
	ATOM	1371	CG2	VAL .	A	243	51.497	32.842	15.109	1.00	48.50	A
	MOTA	1372	C	VAL .	A	243	49.150	30.342	13.389	1.00	44.12	A
45	MOTA	1373	0	VAL .	A	243	48.956	30.765	12.247	1.00	44.46	A
	MOTA	1374	N	GLY .	A	244	48.348	29.467	13.985	1.00	40.48	A
	ATOM	1375	CA	GLY .	Α	244	47.176	28.941	13.306	1.00	37.65	A
	ATOM	1376	С	GLY .	A	244	46.101	29.960	12.964	1.00	35.39	A
	MOTA	1377	0	GLY .			46.313	31.168	13.065	1.00		A
50	MOTA	1378	N	THR .			44.936	29.463	12.560	1.00		A
	ATOM	1379	CA	THR .			43.813	30.312	12.184	1.00		A
	ATOM	1380	CB	THR .			42.593	29.450	11.829	1.00		A
	ATOM	1381		THR .			42.952	28.573	10.755	1.00		A
	ATOM	1382		THR .			41.419	30.319	11.390	1.00		A
55	ATOM	1383	C	THR .			43.476	31.296	13.296	1.00		A
55	ATOM	1384	0	THR .			43.476	30.907	14.434	1.00		A
	ATOM	1385	N	ALA .			43.486	32.576	12.938	1.00		
			CA.									A
	ATOM	1386		ALA .			43.247	33.675	13.867	1.00		A
	ATOM	1387	CB	ALA .	A	∠46	42.956	34.955	13.082	1.00	44.94	A

	ATOM	1388	C	ALA	Α	246	42.178	33.475	14.934	1.00	21.27	A
	ATOM	1389	0	ALA			42.431	33.705	16.114		20.93	A
	ATOM	1390	N	GLN			40.988	33.047	14.536		19.67	A
	ATOM	1391	CA	GLN			39.911	32.886	15.504		20.17	A
5	ATOM	1392	CB	GLN			38.608	32.535	14.779		21.89	A
,	ATOM	1393	CG	GLN			38.522	33.076	13.355		26.18	A
	ATOM	1394	CD	GLN			37.220	33.794	13.064		27.30	A
											30.13	
	ATOM	1395		GLN			36.172	33.447	13.605			A
10	ATOM	1396	NE2				37.278	34.792	12.189		28.70	A
10	MOTA	1397	С	GLN			40.181	31.849	16.595		19.43	A
	MOTA	1398	0	GLN			39.546	31.883	17.648		18.93	A
	ATOM	1399	N	TYR			41.132	30.948	16.359		18.60	A
	MOTA	1400	CA	TYR			41.441	29.896	17.329		19.20	A
	ATOM	1401	CB	TYR			41.333	28.529	16.642		17.53	A
15	MOTA	1402	CG	TYR	Α	248	40.013	28.362	15.927	1.00	19.32	A
	MOTA	1403	CD1	TYR	Α	248	38.859	28.010	16.625	1.00	17.69	A
	MOTA	1404	CE1	TYR	Α	248	37.617	27.976	15.990	1.00	18.18	A
	MOTA	1405	CD2	TYR	Α	248	39.897	28.664	14.569	1.00	16.87	A
	ATOM	1406	CE2	TYR	Α	248	38.665	28.635	13.924	1.00	19.17	A
20	ATOM	1407	CZ	TYR	Α	248	37.527	28.295	14.643	1.00	19.46	A
	ATOM	1408	OH	TYR	Α	248	36.299	28.311	14.023	1.00	18.98	A
	ATOM	1409	С	TYR	А	248	42.810	30.039	17.993	1.00	20.42	A
	ATOM	1410	ō	TYR			43.208	29.191	18.792		19.19	A
	ATOM	1411	N	VAL			43.523	31.114	17.673		20.20	A
25	ATOM	1412	CA	VAL			44.841	31.343	18.251		20.91	A
	ATOM	1413	CB	VAL			45.542	32.532	17.570		21.18	A
	ATOM	1414		VAL			46.821	32.896	18.317		22.45	A
	ATOM	1415		VAL			45.862	32.170	16.139		24.01	A
	ATOM	1416	C	VAL			44.764	31.606	19.750		21.52	A
30	ATOM	1417	0	VAL				32.368	20.216		22.72	A
30			N				43.915					
	ATOM	1418		SER			45.654	30.965	20.503		20.70	A
	ATOM	1419	CA	SER			45.697	31.133	21.951		21.65	A
	ATOM	1420	CB	SER			46.370	29.919	22.613		22.02	A
	MOTA	1421	OG	SER			47.692	29.725	22.132		22.12	A
35	MOTA	1422	C	SER			46.476	32.402	22.280		22.13	A
	MOTA	1423	0	SER			47.332	32.828	21.511		22.77	A
	MOTA	1424	N	PRO			46.180	33.029	23.425		22.23	A
	MOTA	1425	CD	PRO			45.163	32.684	24.433		22.97	A
	MOTA	1426	CA	PRO			46.893	34.254	23.800		22.52	A
40	MOTA	1427	CB	PRO			46.233	34.650	25.127		23.06	A
	ATOM	1428	CG	PRO			45.726	33.329	25.676		22.55	A
	MOTA	1429	С	PRO			48.414	34.115	23.907		22.15	A
	MOTA	1430	0	PRO	Α	251	49.143	35.047	23.563	1.00	22.62	A
	MOTA	1431	N	GLU	Α	252	48.901	32.966	24.367	1.00	20.69	A
45	MOTA	1432	CA	GLU	Α	252	50.347	32.772	24.500	1.00	21.40	A
	ATOM	1433	CB	GLU	Α	252	50.673	31.382	25.071	1.00	20.59	A
	ATOM	1434	CG	GLU	Α	252	49.993	30.232	24.352	1.00	21.91	A
	ATOM	1435	CD	GLU	Α	252	48.691	29.822	25.014	1.00	21.51	A
	ATOM	1436		GLU			47.989	30.707	25.550		21.46	A
50	ATOM	1437		GLU			48.367	28.613	24.993		20.23	A
	ATOM	1438	С	GLU			51.071	32.970	23.167		22.99	A
	ATOM	1439	ō	GLU			52.191	33.480	23.136		23.17	A
	ATOM	1440	N	LEU			50.441	32.576	22.064		23.00	A
	ATOM	1441	CA	LEU			51.068	32.753	20.758		25.62	A
55	ATOM	1442	CB	LEU			50.277	32.029	19.669		26.75	A
55	ATOM	1443	CG	LEU			50.743	30.620	19.296		31.87	A
				LEU			50.433	29.651	20.422		31.81	
	MOTA	1444										A
	MOTA	1445		LEU			50.044	30.179	18.015		31.86	A
	MOTA	1446	C	LEU	А	203	51.201	34.228	20.371	1.00	26.94	A

	ATOM	1447	0	LEU	А	253	52.107	34.601	19.626	1.00	27.09	A
	ATOM	1448	N	LEU			50.297	35.059	20.877		25.83	A
	ATOM	1449	CA	LEU	А	254	50.297	36.485	20.564	1.00	27.26	A
	ATOM	1450	CB	LEU			48.858	37.006	20.564	1.00	25.84	A
5	ATOM	1451	CG	LEU			47.882	36.290	19.621		24.69	A
	ATOM	1452		LEU			46,459	36.724	19.932		23.64	A
	ATOM	1453		LEU			48.236	36.597	18.177		24.24	A
	ATOM	1454	C	LEU			51.134	37.314	21.537		30.62	A
	ATOM	1455	ō	LEU			51.633	38.383	21.187		32.35	A
10	ATOM	1456	N	THR			51.292	36.821	22.758		32.47	A
	ATOM	1457	CA	THR			52.056	37.547	23.759		36.70	A
	ATOM	1458	CB	THR			51.368	37.478	25.127		34.51	A
	ATOM	1459		THR			51.188	36.106	25.494		35.49	A
	ATOM	1460		THR			50.013	38.166	25.077		33.40	A
15	ATOM	1461	C	THR			53.477	37.035	23.910		40.09	A
13	ATOM	1462	Ö	THR			54.430	37.793	23.772		43.69	A
	ATOM	1463	N	GLU			53.617	35.747	24.189		44.77	A
	ATOM	1464	CA	GLU			54.932	35.144	24.103		49.15	A
	ATOM	1465	CB	GLU			54.866	34.143	25.534		51.24	A
20	ATOM	1466	CG	GLU			54.514	34.786	26.862		56.03	A
20	ATOM	1467	CD	GLU			54.053	33.780	27.893		58.83	A
	ATOM	1468		GLU			54.766	32.776	28.107		62.13	A
	ATOM	1469		GLU			52.979	33.996	28.494		60.34	A
	ATOM	1470	C	GLU			55.475	34.456	23.137		50.09	A
25	ATOM	1471	ō	GLU			56.616	33.995	23.127		50.42	A
	ATOM	1472	N	LYS			54.658	34.389	22.090		51.21	A
	ATOM	1473	CA	LYS			55.064	33.746	20.845		51.22	A
	ATOM	1474	CB	LYS			56.244	34.502	20.227		53.28	A
	ATOM	1475	CG	LYS			56.558	34.125	18.790		55.19	A
30	ATOM	1476	CD	LYS			57.709	34.961	18.253		57.52	A
	ATOM	1477	CE	LYS			57.952	34.694	16.777		58.52	A
	ATOM	1478	NZ	LYS			58.290	33.268	16.515		60.88	A
	ATOM	1479	c	LYS			55.467	32.302	21.138		50.74	A
	ATOM	1480	ō	LYS			56.432	31.790	20.577		52.26	A
35	MOTA	1481	N	SER			54.721	31.654	22.027		48.07	A
	ATOM	1482	CA	SER			54.999	30.273	22.402		46.87	A
	ATOM	1483	СВ	SER			55.590	30.229	23.812		48.88	A
	ATOM	1484	OG	SER			54.741	30.892	24.734		53.14	A
	ATOM	1485	c	SER			53.735	29.415	22.342		44.07	A
40	ATOM	1486	0	SER			52.617	29.932	22.417		44.17	A
	ATOM	1487	N	ALA			53.917	28.105	22.204		38.30	A
	ATOM	1488	CA	ALA	А	259	52.793	27.180	22.127	1.00	34.73	A
	ATOM	1489	CB	ALA	А	259	52.551	26.779	20.684	1.00	34.16	A
	ATOM	1490	С	ALA	Α	259	53.042	25.940	22.977	1.00	32.34	A
45	ATOM	1491	0	ALA	Α	259	54.172	25.459	23.086	1.00	31.81	A
	ATOM	1492	N	CYS	A	260	51.975	25.428	23.579	1.00	28.58	A
	ATOM	1493	CA	CYS	Α	260	52.056	24.244	24.425	1.00	26.27	A
	MOTA	1494	CB	CYS	Α	260	52.183	24.654	25.892	1.00	26.53	A
	MOTA	1495	SG	CYS	Α	260	50.846	25.739	26.469	1.00	32.91	A
50	MOTA	1496	C	CYS	Α	260	50.786	23.435	24.224	1.00	22.83	A
	ATOM	1497	0	CYS	Α	260	49.892	23.856	23.495	1.00	22.14	A
	MOTA	1498	N	LYS	Α	261	50.706	22.277	24.868	1.00	20.02	A
	ATOM	1499	CA	LYS	Α	261	49.526	21.434	24.744	1.00	20.65	A
	MOTA	1500	CB	LYS	A	261	49.619	20.243	25.696	1.00	23.28	A
55	MOTA	1501	CG	LYS	Α	261	50.716	19.253	25.347	1.00	27.44	A
	MOTA	1502	CD	LYS			50.732	18.117	26.350		29.98	A
	MOTA	1503	CE	LYS			51.922	17.203	26.134		32.34	A
	MOTA	1504	NZ	LYS			51.940	16.121	27.153		33.28	A
	MOTA	1505	C	LYS	A	261	48.268	22.229	25.062	1.00	19.20	A

	ATOM	1506	0	LYS	Α	261	47.253	22.092	24.387	1.00	18.08	A
	ATOM	1507	N	SER	А	262	48.358	23.068	26.089	1.00	16.92	A
	ATOM	1508	CA	SER			47.235	23.883	26.534		18.13	A
	MOTA	1509	CB	SER			47.644	24.698	27.770		18.27	A
5	ATOM	1510	OG	SER			46.517	25.258	28.421		22.53	A
	MOTA	1511	C	SER	Α	262	46.736	24.811	25.424	1.00	16.77	A
	ATOM	1512	0	SER	Α	262	45.591	25.254	25.450	1.00	15.69	A
	ATOM	1513	N	SER	А	263	47.595	25.118	24.456	1.00	16.44	A
	ATOM	1514	CA			263	47.175	25.970	23.347		16.89	A
10	ATOM	1515	CB	SER			48.340	26.228	22.382		18.49	A
10												
	MOTA	1516	OG			263	49.402	26.909	23.031		22.10	A
	MOTA	1517	С	SER			46.040	25.257	22.612		17.79	A
	MOTA	1518	0	SER			45.099	25.898	22.148		17.57	A
	ATOM	1519	N	ASP	Α	264	46.119	23.928	22.517	1.00	16.30	A
15	MOTA	1520	CA	ASP	Α	264	45.069	23.166	21.836	1.00	16.72	A
	ATOM	1521	CB	ASP	Α	264	45.483	21.704	21.620	1.00	15.92	A
	ATOM	1522	CG	ASP	Δ	264	46.544	21.539	20.548	1.00	17.93	A
	ATOM	1523		ASP			46.642	22.412	19.661		16.78	A
	ATOM	1524		ASP			47.265	20.515	20.579		16.64	A
20												
20	MOTA	1525	C	ASP			43.773	23.194	22.646		17.67	A
	MOTA	1526	0	ASP			42.681	23.197	22.076		18.27	A
	MOTA	1527	N	LEU			43.898	23.205	23.974		15.49	A
	ATOM	1528	CA	LEU	Α	265	42.730	23.232	24.849	1.00	14.75	A
	ATOM	1529	CB	LEU	Α	265	43.147	23.038	26.313	1.00	11.38	A
25	ATOM	1530	CG	LEU	А	265	43.711	21.641	26.621	1.00	14.04	A
	ATOM	1531		LEU			44.249	21.579	28.052		13.96	A
	ATOM	1532		LEU			42.619	20.603	26.416		11.62	A
			C	LEU								
	MOTA	1533				265	41.999	24.557	24.675		15.13	A
	MOTA	1534	0	LEU			40.777	24.620	24.785		16.75	A
30	MOTA	1535	N	TRP			42.746	25.622	24.405		16.08	A
	MOTA	1536	CA	TRP	Α	266	42.118	26.918	24.184	1.00	16.96	A
	ATOM	1537	CB	TRP	Α	266	43.176	28.015	24.023	1.00	17.28	A
	ATOM	1538	CG	TRP	Α	266	42.618	29.326	23.521	1.00	20.54	A
	ATOM	1539	CD2	TRP	Α	266	42.313	30.490	24.301	1.00	20.07	A
35	MOTA	1540	CE2	TRP	А	266	41.782	31.459	23.417		20.46	A
	ATOM	1541		TRP			42.435	30.810	25.660		20.68	A
	ATOM	1542		TRP			42.270	29.631	22.231		19.53	A
				TRP								
	ATOM	1543					41.769	30.908	22.163		19.61	A
	MOTA	1544		TRP			41.372	32.727	23.850		20.90	A
40	MOTA	1545		TRP			42.026	32.073	26.091		19.45	A
	ATOM	1546	CH2	TRP	Α	266	41.501	33.015	25.185	1.00	20.71	A
	ATOM	1547	С	TRP	Α	266	41.284	26.795	22.913	1.00	17.22	A
	ATOM	1548	0	TRP	Α	266	40.139	27.240	22.863	1.00	18.03	A
	ATOM	1549	N	ALA	А	267	41.863	26.181	21.886	1.00	17.50	A
45	ATOM	1550	CA	ALA			41.155	25.990	20.626		16.16	A
	ATOM	1551	CB	ALA			42.050	25.290	19.621		14.28	A
	ATOM	1552	С	ALA			39.901	25.159	20.891		16.28	A
	MOTA	1553	0	ALA			38.835	25.436	20.346		16.46	A
	MOTA	1554	N	LEU			40.031	24.144	21.739		16.57	A
50	MOTA	1555	CA	LEU	Α	268	38.890	23.299	22.084	1.00	17.03	A
	ATOM	1556	CB	LEU	Α	268	39.292	22.260	23.139	1.00	15.35	A
	MOTA	1557	CG	LEU	Α	268	38.158	21.429	23.754	1.00	19.00	A
	ATOM	1558	CD1	LEU	Α	268	37.505	20.578	22.678		16.17	A
	ATOM	1559		LEU			38.718	20.537	24.881		17.49	A
55	ATOM	1560	C	LEU			37.766	24.179	22.628		15.72	A
55			0									
	MOTA	1561		LEU			36.603	24.031	22.247		15.28	A
	ATOM	1562	N			269	38.119	25.099	23.520		14.34	A
	MOTA	1563	CA	GLY			37.124	25.989	24.092		13.39	A
	MOTA	1564	C	GLY	Α	269	36.406	26.808	23.031	1.00	14.94	A

	ATOM	1565	0	GLY .	A	269	35.193	27.014	23.114	1.00	14.76	A
	ATOM	1566	N	CYS .	Α	270	37.146	27.279	22.030	1.00	13.86	A
	ATOM	1567	CA	CYS .	Α	270	36.539	28.061	20.958	1.00	16.80	A
	ATOM	1568	CB	CYS .	Α	270	37.611	28.634	20.023	1.00	15.97	A
5	ATOM	1569	SG	CYS .	Α	270	38.751	29.810	20.780	1.00	20.48	A
	ATOM	1570	С	CYS .	A	270	35.598	27.175	20.140	1.00	17.50	A
	ATOM	1571	0	CYS .	Α	270	34.516	27,604	19.741	1.00	18.38	A
	ATOM	1572	N	ILE .	A	271	36.022	25.939	19.887	1.00	16.99	A
	ATOM	1573	CA	ILE .			35.221	25.004	19.104		16.66	A
10	ATOM	1574	CB	ILE .			36.038	23.741	18.778		16.53	A
	ATOM	1575		ILE .			35.155	22.694	18.102		16.34	A
	ATOM	1576		ILE .			37.222	24.129	17.882		15.59	A
	ATOM	1577		ILE .			38.239	23.018	17.690		14.88	A
	ATOM	1578	C	ILE .			33.920	24.626	19.809	1.00	16.74	A
15	ATOM	1579	o	ILE .			32.865	24.576	19.179		17.12	A
	ATOM	1580	N	ILE .			33.990	24.357	21.111		16.13	A
	ATOM	1581	CA	ILE .	Α	272	32.785	24.021	21.862	1.00	18.30	A
	ATOM	1582	CB	ILE .	A	272	33.097	23.747	23.346	1.00	17.77	A
	ATOM	1583		ILE .			31.796	23.666	24.152		17.96	A
20	ATOM	1584		ILE .			33.877	22.437	23.481		19.55	A
	ATOM	1585	CD1	ILE .	A	272	34.446	22.217	24.886	1.00	18.64	A
	ATOM	1586	C	ILE .	А	272	31.824	25.207	21.776	1.00	19.51	A
	ATOM	1587	0	ILE .	A	272	30.624	25.037	21.554	1.00	20.44	A
	ATOM	1588	N	TYR .	A	273	32.362	26.409	21.947	1.00	18.52	A
25	ATOM	1589	CA	TYR .	A	273	31.553	27.615	21.881	1.00	20.48	A
	ATOM	1590	CB	TYR .	A	273	32.418	28.847	22.162	1.00	18.98	A
	MOTA	1591	CG	TYR .	Α	273	31.663	30.161	22.125	1.00	20.26	A
	ATOM	1592	CD1	TYR .	А	273	31.229	30.709	20.916	1.00	20.67	A
	ATOM	1593	CE1	TYR .	Α	273	30.536	31.917	20.880	1.00	20.98	A
30	ATOM	1594	CD2	TYR .	Α	273	31.383	30.857	23.302	1.00	19.82	A
	ATOM	1595	CE2	TYR .	Α	273	30.691	32.062	23.280	1.00	20.62	A
	ATOM	1596	CZ	TYR .	Α	273	30.271	32.587	22.067	1.00	21.15	A
	MOTA	1597	OH	TYR .	A	273	29.588	33.776	22.049	1.00	21.86	A
	MOTA	1598	C	TYR .	A	273	30.902	27.730	20.507	1.00	21.54	A
35	ATOM	1599	0	TYR .	Α	273	29.719	28.049	20.401	1.00	22.80	A
	ATOM	1600	N	GLN .	A	274	31.676	27.454	19.461	1.00	21.05	A
	MOTA	1601	CA	GLN .	Α	274	31.176	27.538	18.095	1.00	21.48	A
	MOTA	1602	CB	GLN .	Α	274	32.323	27.341	17.097	1.00	21.41	A
	ATOM	1603	CG	GLN .	A	274	31.934	27.596	15.645	1.00	23.15	A
40	ATOM	1604	CD	GLN .	Α	274	33.131	27.588	14.706	1.00	24.80	A
	ATOM	1605	OE1	GLN .	Α	274	34.276	27.446	15.139	1.00	22.51	A
	MOTA	1606	NE2	GLN .	Α	274	32.870	27.750	13.413	1.00	22.96	A
	MOTA	1607	C	GLN .	A	274	30.076	26.517	17.828	1.00	21.51	A
	MOTA	1608	0	GLN .	A	274	29.123	26.806	17.108	1.00	20.50	A
45	MOTA	1609	N	LEU .	A	275	30.207	25.324	18.403	1.00	21.44	A
	MOTA	1610	CA	LEU .	A	275	29.196	24.282	18.208	1.00	20.95	A
	MOTA	1611	CB	LEU .	A	275	29.645	22.958	18.846	1.00	19.11	A
	MOTA	1612	CG	LEU .			30.775	22.182	18.159		21.43	A
	MOTA	1613		LEU .			31.118	20.936	18.963	1.00	17.64	A
50	MOTA	1614	CD2	LEU .	A	275	30.342	21.795	16.754	1.00	20.34	A
	MOTA	1615	C	LEU .			27.860	24.697	18.815		21.32	A
	MOTA	1616	0	LEU .			26.802	24.461	18.229	1.00	19.75	A
	MOTA	1617	N	VAL .			27.921	25.322	19.987		19.10	A
	MOTA	1618	CA	VAL .			26.724	25.750	20.702		22.47	A
55	MOTA	1619	CB	VAL .			27.011	25.882	22.217		20.87	A
	MOTA	1620		VAL .			25.742	26.291	22.957		19.68	A
	MOTA	1621					27.550	24.558	22.766		19.43	A
	MOTA	1622	C	VAL .			26.127	27.075	20.211		23.89	A
	MOTA	1623	0	VAL .	A	276	24.910	27.199	20.070	1.00	24.90	A

	ATOM	1624	N	ALA	-	277	26.983	28.062	19.965	1 00	24.56	А
	MOTA	1625	CA	ALA			26.533	29.374	19.518		24.72	A
	ATOM	1626	CB	ALA	Α	277	27.504	30.444	19.999	1.00	24.36	A
	ATOM	1627	С	ALA	А	277	26.378	29.458	18.005	1.00	25.76	A
5	ATOM	1628		ALA			25.577	30.242	17.502		26.39	A
,			0									
	MOTA	1629	N	GLY	Α	278	27.142	28.651	17.280	1.00	25.13	A
	ATOM	1630	CA	GLY	Α	278	27.062	28.673	15.834	1.00	25.58	A
	ATOM	1631	С	GLY	А	278	28.163	29.524	15.231	1.00	26.50	A
	ATOM	1632	ō	GLY			28.374	29.510	14.015		28.17	A
10												
10	MOTA	1633	N	LEU			28.866	30.262	16.086		24.44	A
	MOTA	1634	CA	LEU			29.962	31.130	15.656	1.00	25.21	A
	ATOM	1635	CB	LEU	Α	279	29.468	32.575	15.500	1.00	25.78	A
	MOTA	1636	CG	LEU	А	279	28.364	32.899	14.490	1.00	28.17	A
	ATOM	1637		LEU			27.922	34.344	14.684		26.60	A
1.5												
15	MOTA	1638		LEU			28.862	32.670	13.071		26.52	A
	MOTA	1639	C	LEU	Α	279	31.093	31.116	16.687	1.00	23.47	A
	ATOM	1640	0	LEU	Α	279	30.848	30.994	17.882	1.00	24.44	A
	MOTA	1641	N	PRO	А	280	32.349	31.239	16.236	1.00	23.35	A
	ATOM	1642	CD	PRO			32.831	31.404	14.855		22.26	A
20												
20	MOTA	1643	CA	PRO			33.464	31.239	17.189		23.81	A
	MOTA	1644	CB	PRO	Α	280	34.692	31.293	16.282	1.00	23.24	A
	ATOM	1645	CG	PRO	Α	280	34.189	32.020	15.073	1.00	24.89	A
	ATOM	1646	C	PRO	А	280	33.353	32.444	18.137	1.00	22.69	A
	ATOM	1647	ō	PRO			32.750	33.457	17.788		22.11	A
25												
25	MOTA	1648	N	PRO			33.939	32.344	19.345		23.06	A
	MOTA	1649	CD	PRO			34.810	31.223	19.734		21.37	A
	ATOM	1650	CA	PRO	Α	281	33.935	33.375	20.395	1.00	23.67	A
	MOTA	1651	CB	PRO	А	281	34.781	32.751	21.509	1.00	24.89	A
	ATOM	1652	CG	PRO			34.749	31.287	21.219		25.24	A
30								34.752			23.75	
30	MOTA	1653	C	PRO			34.481		20.017			A
	MOTA	1654	0	PRO			33.869	35.781	20.317		21.02	A
	MOTA	1655	N	PHE	Α	282	35.644	34.763	19.379	1.00	22.17	A
	MOTA	1656	CA	PHE	Α	282	36.293	36.007	18.998	1.00	23.16	A
	ATOM	1657	CB	PHE			37.765	35.943	19.406		21.01	A
35		1658		PHE							22.66	
33	MOTA		CG				37.975	35.482	20.822			A
	ATOM	1659		PHE			37.806	36.361	21.888		20.06	A
	MOTA	1660	CD2	PHE	Α	282	38.291	34.151	21.093	1.00	20.72	A
	MOTA	1661	CE1	PHE	Α	282	37.947	35.921	23.206	1.00	22.66	A
	ATOM	1662	CE2	PHE	Δ	282	38.433	33.702	22.405	1 00	20.97	A
40	ATOM	1663	CZ	PHE			38.261	34.590	23.466		19.58	A
40												
	MOTA	1664	C	PHE			36.169	36.263	17.503		24.39	A
	MOTA	1665	0	PHE	Α	282	36.802	35.585	16.694	1.00	25.80	A
	ATOM	1666	N	ARG	Α	283	35.355	37.248	17.142	1.00	24.99	A
	MOTA	1667	CA	ARG	А	283	35.141	37.594	15.741	1.00	26.33	A
45	ATOM	1668	CB	ARG			33.721	37.209	15.316		28.91	A
75												
	MOTA	1669	CG	ARG			33.293	35.808	15.724		30.27	A
	MOTA	1670	CD	ARG			31.904	35.493	15.188		33.36	A
	MOTA	1671	NE	ARG	Α	283	30.890	36.392	15.733	1.00	32.76	A
	ATOM	1672	CZ	ARG	Α	283	30.372	36.287	16.952	1.00	34.79	A
50	ATOM	1673		ARG			30.767	35.317	17.768		35.77	A
50												
	MOTA	1674		ARG			29.458	37.156	17.359		36.12	A
	MOTA	1675	C	ARG			35.328	39.096	15.544		26.47	A
	MOTA	1676	0	ARG	Α	283	35.029	39.888	16.438	1.00	26.28	A
	MOTA	1677	N	ALA	Α	284	35.818	39.486	14.373	1.00	26.70	A
55	ATOM	1678	CA	ALA			36.033	40.899	14.079		27.84	A
22			CB									
	MOTA	1679		ALA			37.188	41.442	14.914		26.24	A
	MOTA	1680	C	ALA			36.327	41.077	12.602		28.35	A
	MOTA	1681	0	ALA			36.560	40.101	11.891		29.91	A
	MOTA	1682	N	$\operatorname{GL} Y$	Α	285	36.332	42.329	12.153	1.00	29.29	A

	ATOM	1683	CA	GLY	А	285	36.577	42.631	10.753	1.00	29.52	A
	ATOM	1684	C	GLY			37,893	42.156	10.168		30.12	A
	ATOM	1685	ō	GLY			37.974	41.862	8.976		30.60	A
	ATOM	1686	N	ASN			38.939	42.097	10.983		28.49	A
5	ATOM	1687	CA	ASN			40.231	41.644	10.489		26.71	A
,	ATOM	1688	CB	ASN			41.050	42.825	9.945		26.11	A
	ATOM	1689	CG	ASN			41.310	43.900	10.990		27.83	A
											27.84	
	ATOM	1690		ASN			41.877	43.631	12.049			A
10	ATOM	1691		ASN			40.908	45.131	10.685		25.95	A
10	MOTA	1692	С	ASN			40.997	40.924	11.584		26.03	A
	MOTA	1693	0	ASN			40.540	40.851	12.723		25.66	A
	MOTA	1694	N	GLU			42.162	40.391	11.239		24.81	A
	MOTA	1695	CA	GLU			42.965	39.662	12.206		27.59	A
	ATOM	1696	CB	GLU			44.145	38.985	11.510		30.17	A
15	ATOM	1697	CG	GLU			43.776	37.632	10.931		38.21	A
	MOTA	1698	CD	GLU	Α	287	44.900	36.998	10.140	1.00	41.86	A.
	MOTA	1699	OE1	GLU	Α	287	46.061	37.036	10.608	1.00	43.08	A
	ATOM	1700	OE2	GLU	Α	287	44.612	36.449	9.052	1.00	45.22	A
	MOTA	1701	C	GLU	Α	287	43.459	40.485	13.383	1.00	25.05	A
20	ATOM	1702	0	GLU	Α	287	43.382	40.030	14.521	1.00	26.41	A
	ATOM	1703	N	TYR	Α	288	43.966	41.685	13.122	1.00	23.04	A
	ATOM	1704	CA	TYR			44.460	42.528	14.205	1.00	22.34	A
	ATOM	1705	CB	TYR			44.867	43.913	13.691		21.07	A
	ATOM	1706	CG	TYR			45.275	44.858	14.805		21.07	A
25	ATOM	1707		TYR			46.533	44.762	15.405		21.23	A
	ATOM	1708	CE1	TYR			46.891	45.588	16.475		20.43	A
	ATOM	1709	CD2	TYR			44.380	45.809	15.302		22.32	A
	ATOM	1710	CE2	TYR			44.725	46.637	16.373		23.28	A
	ATOM	1711	CZ	TYR			45.981	46.518	16.953		22.96	A
30	ATOM	1711	OH	TYR			46.316	47.313	18.024		23.18	A
30			C									A
	MOTA	1713		TYR			43.402	42.698	15.288		21.38	
	ATOM	1714	0	TYR			43.710	42.616	16.473		22.09	A
	ATOM	1715	N	LEU			42.159	42.939	14.874		21.88	A
	ATOM	1716	CA	LEU			41.055	43.130	15.811		21.98	A
35	MOTA	1717	CB	LEU			39.821	43.673	15.078		22.90	A
	MOTA	1718	CG	LEU			39.896	45.130	14.601		26.52	A
	MOTA	1719		LEU			38.706	45.436	13.696		26.55	A
	MOTA	1720		LEU			39.914	46.071	15.807		23.13	A
	MOTA	1721	C	LEU			40.686	41.849	16.560		21.24	A
40	MOTA	1722	0	LEU			40.256	41.897	17.715		20.72	A.
	MOTA	1723	N	ILE			40.843	40.708	15.900		19.62	A
	MOTA	1724	CA	ILE			40.538	39.433	16.533		18.54	A
	MOTA	1725	CB	ILE	Α	290	40.560	38.281	15.509	1.00	18.52	A
	MOTA	1726	CG2	ILE	Α	290	40.503	36.934	16.234	1.00	17.63	A
45	MOTA	1727	CG1	ILE	Α	290	39.378	38.429	14.545	1.00	18.88	A
	ATOM	1728	CD1	ILE	Α	290	39.421	37.483	13.357	1.00	19.81	A
	ATOM	1729	С	ILE	Α	290	41.578	39.167	17.618	1.00	19.09	A
	ATOM	1730	0	ILE	Α	290	41.236	38.788	18.737	1.00	18.20	A
	ATOM	1731	N	PHE			42.849	39.376	17.286		18.76	A
50	ATOM	1732	CA	PHE			43.925	39.156	18.247		20.75	A
	ATOM	1733	CB	PHE			45.286	39.434	17.606		20.71	A
	ATOM	1734	CG	PHE			45.644	38.480	16.503		22.92	A
	ATOM	1735		PHE			45.065	37.214	16.443		22.98	A
	ATOM	1736	CD2				46.588	38.830	15.543		22.91	A
55	ATOM	1737		PHE			45.423	36.310	15.440		24.51	A
33			CE2									
	MOTA	1738					46.954	37.931	14.535		25.54	A
	MOTA	1739	CZ	PHE			46.370	36.670	14.485		23.29	A
	ATOM	1740	С	PHE			43.739	40.061	19.451		21.72	A
	MOTA	1741	0	PHE	A	291	43.992	39.671	20.593	1.00	22.32	A

	a moar	1742	NT.	GLN	20	202	43.284	41.275	19.178	1 00	23.27	70
	MOTA	1742	N									A
	MOTA	1743	CA	GLN	А	292	43.055	42.264	20.216		24.01	A
	ATOM	1744	CB	GLN	Α	292	42.574	43.559	19.562	1.00	25.77	A
	ATOM	1745	CG	GLN	Δ	292	42.577	44.773	20.447		28.45	A
5												
3	MOTA	1746	CD	GLN			42.469	46.057	19.638		29.83	A
	MOTA	1747	OE1	GLN	Α	292	41.520	46.244	18.872		27.16	A
	ATOM	1748	NE2	GLN	А	292	43.449	46.944	19.799	1.00	27.61	A
	ATOM	1749	С	GLN	Δ	292	42.018	41.733	21.204	1 00	22.97	A
	ATOM	1750	o	GLN			42.200	41.832	22.415		21.64	A
10	MOTA	1751	N	LYS			40.937	41.154	20.687		21.82	A
	MOTA	1752	CA	LYS	Α	293	39.895	40.612	21.558	1.00	22.18	A
	ATOM	1753	CB	LYS	Α	293	38.664	40.223	20.740	1.00	22.69	A
	ATOM	1754	CG	LYS			37.919	41.407	20.153		25.78	A
	ATOM	1755	CD	LYS			36.651	40.961	19.429		27.88	A
15	MOTA	1756	CE	LYS			35.857	42.161	18.926		30.85	A
	MOTA	1757	NZ	LYS	Α	293	34.612	41.750	18.214	1.00	32.98	A
	ATOM	1758	C	LYS	Α	293	40.398	39.398	22.343	1.00	21.20	A
	MOTA	1759	0	LYS	А	293	40.041	39.204	23.509	1.00	22.01	A
	ATOM	1760	N	ILE			41.226	38.583	21.702		19.91	A
20												
20	MOTA	1761	CA	ILE			41.774	37.394	22.347		20.28	A
	ATOM	1762	CB	ILE	Α	294	42.631	36.575	21.349	1.00	18.98	A
	ATOM	1763	CG2	ILE	Α	294	43.481	35.550	22.098	1.00	17.70	A
	ATOM	1764	CG1	ILE	А	294	41.716	35.897	20.318	1.00	17.93	A
	ATOM	1765		ILE			42.467	35.237	19.178		16.21	A
25											21.94	
23	MOTA	1766	C	ILE			42.618	37.727	23.587			A
	MOTA	1767	0	ILE			42.366	37.199	24.673		20.86	A
	ATOM	1768	N	ILE	Α	295	43.610	38.600	23.439	1.00	21.88	A
	ATOM	1769	CA	ILE	Α	295	44.461	38.934	24.582	1.00	24.25	A
	ATOM	1770	CB	ILE			45.668	39.805	24.175		23.93	A
30												
30	MOTA	1771	CG2				46.514	39.066	23.140		24.61	A
	MOTA	1772		ILE			45.189	41.151	23.637		24.58	A
	ATOM	1773	CD1	ILE	Α	295	46.317	42.149	23.433	1.00	26.69	A
	MOTA	1774	C	ILE	Α	295	43.720	39.636	25.717	1.00	24.80	A
	ATOM	1775	0	ILE			44.214	39.687	26.842		24.76	A
35	ATOM	1776	N	LYS			42.539	40.173	25.425		25.33	A
33												
	MOTA	1777	CA	LYS			41.743	40.853	26.444		26.80	A
	MOTA	1778	CB	LYS			41.178	42.170	25.894		27.39	A
	ATOM	1779	CG	LYS	Α	296	42.240	43.141	25.413	1.00	31.79	A
	MOTA	1780	CD	LYS	А	296	41.634	44.410	24.826	1.00	35.56	A
40	ATOM	1781	CE	LYS			41.009	45.283	25.900		39.29	A
40												
	MOTA	1782	NZ	LYS			40.564	46.603	25.357		41.72	A
	MOTA	1783	С	LYS			40.593	39.958	26.893		25.50	A
	ATOM	1784	0	LYS	Α	296	39.770	40.361	27.713	1.00	24.02	A
	ATOM	1785	N	LEU	Α	297	40.550	38.742	26.349	1.00	25.67	A
45	ATOM	1786	CA	LEU			39.500	37.777	26.666		25.16	A
	ATOM	1787	CB	LEU			39.632	37.285	28.111		24.80	A
	MOTA	1788	CG	LEU			38.766	36.068	28.460		26.43	A
	ATOM	1789	CD1	LEU	Α	297	39.238	34.852	27.646	1.00	26.70	A
	ATOM	1790	CD2	LEU	Α	297	38.856	35.777	29.951	1.00	24.84	A
50	ATOM	1791	C	LEU			38.151	38.459	26.467		25.11	A
50	ATOM	1792	ō	LEU			37.261	38.378	27.309		25.28	A
	MOTA	1793	N	GLU			38.007	39.127	25.331		24.98	A
	MOTA	1794	CA	GLU	Α	298	36.786	39.847	25.023	1.00	25.31	A
	MOTA	1795	CB	GLU	Α	298	37.143	41.139	24.291	1.00	27.13	A
55	ATOM	1796	CG	GLU			35.991	42.092	24.108		31.28	A
22			CD									
	MOTA	1797		GLU			36.419	43.362	23.410		34.40	A
	MOTA	1798		GLU			37.348	44.027	23.918		35.90	A
	MOTA	1799	OE2	GLU			35.832	43.693	22.359		36.16	A
	MOTA	1800	C	GLU	Α	298	35.766	39.057	24.207	1.00	23.79	A

	ATOM	1801	0	GLU	Α	298	35.832	39.017	22.979	1.00 2	4.35	A
	ATOM	1802	N			299	34.825	38.427	24.902	1.00 2		A
	ATOM	1803	CA			299	33.760	37.663	24.265	1.00 2		A
	ATOM	1804	CB			299	34.264	36.304	23.755	1.00 2		A
5	ATOM	1805	CG			299	34.348	35.233	24.828	1.00 2		A
,	ATOM	1806		TYR			35.336	35.279	25.810	1.00 2		A
	ATOM	1807		TYR			35.389	34.332	26.826	1.00 1		
												A
	ATOM	1808		TYR			33.410	34.201	24.888	1.00 1		A
	MOTA	1809	CE2	TYR			33.456	33.243	25.907	1.00 1		A
10	MOTA	1810	CZ			299	34.449	33.321	26.870	1.00 1		A
	MOTA	1811	OH			299	34.511	32.401	27.881	1.00 1		A
	ATOM	1812	С			299	32.699	37.437	25.331	1.00 2		A
	MOTA	1813	0			299	32.942	37.681	26.506	1.00 2		A
	ATOM	1814	N	ASP	Α	300	31.522	36.981	24.927	1.00 2	6.94	A
15	MOTA	1815	CA	ASP	Α	300	30.467	36.710	25.891	1.00 3	0.60	A.
	MOTA	1816	CB	ASP	Α	300	29.665	37.981	26.179	1.00 3	5.86	A.
	ATOM	1817	CG	ASP	Α	300	29.228	38.687	24.923	1.00 4	2.04	A
	ATOM	1818	OD1	ASP	Α	300	28.450	38.088	24.149	1.00 4	5.98	A
	ATOM	1819	OD2	ASP	Α	300	29.666	39.840	24.707	1.00 4	5.69	A
20	ATOM	1820	C	ASP	Α	300	29.564	35.608	25.363	1.00 2	9.26	A
	ATOM	1821	0	ASP	Α	300	29.590	35.299	24.172	1.00 2	8.64	A
	ATOM	1822	N	PHE	А	301	28.778	35.011	26.253	1.00 2	8.96	A
	ATOM	1823	CA			301	27.884	33.924	25.871	1.00 3		A
	ATOM	1824	CB			301	27.818	32.854	26.968	1.00 2		A
25	ATOM	1825	CG			301	29.147	32.279	27.356	1.00 2		A
	ATOM	1826		PHE			29.978	32.949	28.245	1.00 2		A
	ATOM	1827		PHE			29.560	31.050	26.845	1.00 2		A
	ATOM	1828		PHE			31.205	32.403	28.625	1.00 2		A
	ATOM	1829		PHE			30.781	30.498	27.217	1.00 2		A
30			CZ			301		31.175	28.110	1.00 2		A
30	ATOM	1830					31.605					
	ATOM	1831	C			301	26.459	34.384	25.619	1.00 3		A
	ATOM	1832	0			301	25.946	35.261	26.317	1.00 3		A
	MOTA	1833	N			302	25.798	33.804	24.607	1.00 3		A
	MOTA	1834	CD			302	26.313	32.943	23.529	1.00 3		A
35	ATOM	1835	CA			302	24.415	34.199	24.341	1.00 3		A
	ATOM	1836	CB			302	24.144	33.608	22.959	1.00 3		A
	MOTA	1837	CG			302	25.041	32.413	22.921	1.00 3		A
	MOTA	1838	C			302	23.567	33.561	25.444	1.00 3		A
	MOTA	1839	0			302	23.935	32.518	25.986	1.00 3		A
40	MOTA	1840	N			303	22.447	34.188	25.783	1.00 3		A
	MOTA	1841	CA	ALA	Α	303	21.572	33.692	26.843	1.00 4	0.65	A
	MOTA	1842	CB	ALA	Α	303	20.280	34.506	26.862	1.00 4	1.66	A
	MOTA	1843	C	ALA	Α	303	21.238	32.197	26.814	1.00 4	1.25	A
	ATOM	1844	0	ALA	Α	303	21.253	31.537	27.854	1.00 4	3.16	A
45	ATOM	1845	N	ALA	Α	304	20.945	31.665	25.631	1.00 4	1.04	A
	ATOM	1846	CA	ALA	Α	304	20.569	30.258	25.480	1.00 4	0.66	A
	ATOM	1847	CB	ALA	Α	304	20.121	30.004	24.040	1.00 4	1.36	A
	ATOM	1848	С	ALA			21.628	29.223	25.876	1.00 3		A
	MOTA	1849	0	ALA			21.298	28.156	26.395	1.00 4		A
50	ATOM	1850	N			305	22.891	29.543	25.617	1.00 3		A
	ATOM	1851	CA			305	24.022	28.662	25.909	1.00 3		A
	ATOM	1852	CB			305	25.259	29.519	26.187	1.00 2		A
	ATOM	1853	CG			305	26.536	28.917	25.690	1.00 2		A
	ATOM	1854		PHE			27.146	27.875	26.377	1.00 2		A
55	ATOM	1855		PHE			27.146	29.386	24.521	1.00 2		A
23	ATOM	1856		PHE			28.330	27.308	25.908	1.00 2		
		1856	CE2			305				1.00 2		A A
	MOTA	1857	CE2				28.312	28.826	24.042			
	ATOM					305	28.914	27.786	24.737	1.00 2		A
	ATOM	1859	C	PHE	Α	305	23.811	27.664	27.057	1.00 3	0.09	A

	ATOM	1860	0	PHE	Α	305	23.518	28.051	28.187	1.00	31.51	A
	ATOM	1861	N	PHE	Α	306	23.964	26.378	26.758	1.00	27.01	A
	MOTA	1862	CA	PHE	Α	306	23.801	25.334	27.769	1.00	26.30	A
	ATOM	1863	CB	PHE	Α	306	24.157	23.970	27.170	1.00	25.03	A
5	ATOM	1864	CG	PHE	Α	306	23.548	23.725	25.815	1.00	27.24	A
	MOTA	1865	CD1	PHE	Α	306	22.170	23.831	25.622	1.00	28.40	A
	ATOM	1866	CD2	PHE	Α	306	24.350	23.386	24.728	1.00	27.84	A
	ATOM	1867	CE1	PHE	Α	306	21.601	23.603	24.365	1.00	28.05	A
	ATOM	1868	CE2	PHE	Α	306	23.792	23.155	23.465	1.00	28.31	A
10	ATOM	1869	CZ	PHE	Α	306	22.415	23.263	23.283	1.00	28.00	A
	ATOM	1870	C	PHE	А	306	24.711	25.652	28.961	1.00	26.23	A
	ATOM	1871	0	PHE	Α	306	25.927	25.775	28.811	1.00	25.59	A
	ATOM	1872	N	PRO	Α	307	24.125	25.796	30.163	1.00	26.67	A
	ATOM	1873	CD	PRO	Α	307	22.685	25.625	30.430	1.00	27.95	A
15	ATOM	1874	CA	PRO	Α	307	24.842	26.110	31.405	1.00	26.59	A
	ATOM	1875	CB	PRO	Α	307	23.795	25.832	32.481	1.00	26.14	A
	MOTA	1876	CG	PRO	Α	307	22.531	26.250	31.803	1.00	27.86	A
	MOTA	1877	C	PRO	Α	307	26.145	25.355	31.659	1.00	25.58	A
	ATOM	1878	0	PRO	Α	307	27.189	25.964	31.900	1.00	22.65	A
20	ATOM	1879	N	LYS	Α	308	26.085	24.031	31.620	1.00	24.46	A
	ATOM	1880	CA	LYS	Α	308	27.274	23.232	31.867	1.00	23.91	A
	MOTA	1881	CB	LYS	Α	308	26.887	21.760	32.024	1.00	23.25	A
	ATOM	1882	CG	LYS	Α	308	26.062	21.532	33.285	1.00	28.49	A
	ATOM	1883	CD	LYS	Α	308	25.618	20.093	33.466	1.00	30.17	A
25	ATOM	1884	CE	LYS	Α	308	24.760	19.973	34.722	1.00	33.12	A
	ATOM	1885	NZ	LYS	Α	308	24.122	18.636	34.860	1.00	34.13	A
	MOTA	1886	C	LYS	Α	308	28.314	23.426	30.769	1.00	22.84	A
	MOTA	1887	0	LYS	Α	308	29.514	23.411	31.042	1.00	22.46	A
	ATOM	1888	N	ALA	Α	309	27.861	23.621	29.534	1.00	21.59	A
30	MOTA	1889	CA	ALA	Α	309	28.792	23.848	28.432	1.00	20.02	A
	ATOM	1890	CB	ALA	Α	309	28.056	23.856	27.106	1.00	18.80	A
	MOTA	1891	C	ALA	Α	309	29.481	25.191	28.662	1.00	21.41	A
	MOTA	1892	0	ALA			30.680	25.335	28.427		21.39	A
	MOTA	1893	N	ARG			28.717	26.179	29.121		21.39	A
35	ATOM	1894	CA	ARG			29.290	27.494	29.388		22.02	A
	MOTA	1895	CB	ARG			28.213	28.479	29.854	1.00	22.39	A
	MOTA	1896	CG	ARG			28.806	29.756	30.436		25.30	A
	MOTA	1897	CD	ARG			27.780	30.852	30.664		28.33	A
	MOTA	1898	NE	ARG			28.420	32.039	31.230		30.18	A
40	MOTA	1899	CZ	ARG			27.901	33.263	31.203		32.07	A
	MOTA	1900		ARG			26.719	33.477	30.634		31.19	A
	MOTA	1901		ARG			28.567	34.277	31.742		30.49	A
	ATOM	1902	С	ARG			30.376	27.388	30.458		21.65	A
	MOTA	1903	0	ARG			31.464	27.949	30.311		20.36	A
45	MOTA	1904	N	ASP			30.074	26.677	31.541		19.57	A
	MOTA	1905	CA	ASP			31.043	26.512	32.615		20.18	A
	MOTA	1906	CB	ASP			30.460	25.649	33.739		20.39	A
	MOTA	1907	CG	ASP			31.439	25.446	34.881		23.35	A
	MOTA	1908		ASP			32.158	24.428	34.885		24.91	A
50	MOTA	1909		ASP			31.500	26.312	35.776		26.96	A
	MOTA	1910	C			311	32.322	25.877	32.073		19.73	A
	MOTA	1911	0	ASP			33.422	26.289	32.439		19.30	A
	MOTA	1912	N			312	32.179	24.891	31.188		16.32	A
	MOTA	1913	CA	LEU			33.349	24.226	30.611		16.66	A
55	MOTA	1914	CB	LEU			32.927	23.035	29.744		16.12	A
	MOTA	1915	CG			312	34.050	22.320	28.974		14.73	A
	ATOM	1916		LEU			35.192	21.935	29.912		14.56	A
	MOTA	1917		LEU			33.477	21.084	28.289		14.22	A
	MOTA	1918	C	LEU	Α	312	34.181	25.189	29.774	1.00	16.61	A

	ATOM	1919	0	LEU	А	312	35.402	25.241	29.910	1.00	16.20	A
	ATOM	1920	N	VAL			33.515	25.949	28.908		16.20	A
	ATOM	1921	CA	VAL			34.207	26.907	28.058		15.37	A
	ATOM	1922	CB	VAL			33.216	27.648	27.130		16.42	A
5	ATOM	1923		VAL			33.915	28.796	26.426		16.93	A
,	ATOM	1924		VAL			32.644	26.672	26.103		17.88	A
		1924	C	VAL			34.960		28.911		17.39	
	ATOM							27.923				A
	MOTA	1926	0	VAL			36.093	28.294	28.591		18.00	A
10	MOTA	1927	N	GLU			34.342	28.364	30.004		17.61	A
10	MOTA	1928	CA	GLU			34.986	29.331	30.885		20.43	A
	MOTA	1929	CB	GLU			34.009	29.816	31.959		22.14	A
	ATOM	1930	CG	GLU			32.800	30.550	31.396		26.52	A
	MOTA	1931	CD	GLU			31.852	31.025	32.478		31.26	A
	MOTA	1932		GLU			31.580	30.246	33.417		33.48	A
15	MOTA	1933		GLU			31.370	32.173	32.387		34.81	A
	ATOM	1934	C	GLU			36.217	28.721	31.539		19.15	A
	ATOM	1935	0	GLU			37.134	29.433	31.934		21.47	A
	MOTA	1936	N	LYS			36.245	27.400	31.651		19.51	A
	MOTA	1937	CA	LYS	Α	315	37.394	26.749	32.258	1.00	19.17	A
20	ATOM	1938	CB	LYS			36.946	25.514	33.043	1.00	18.84	A
	MOTA	1939	CG	LYS	Α	315	36.280	25.885	34.368	1.00	19.62	A
	ATOM	1940	CD	LYS	Α	315	35.653	24.696	35.073	1.00	19.22	A
	ATOM	1941	CE	LYS	Α	315	35.070	25.095	36.427	1.00	21.00	A
	ATOM	1942	NZ	LYS	Α	315	36.119	25.552	37.381	1.00	19.53	A
25	ATOM	1943	C	LYS	Α	315	38.452	26.393	31.218	1.00	18.96	A
	ATOM	1944	0	LYS	Α	315	39.511	25.873	31.561	1.00	19.85	A
	ATOM	1945	N	LEU	А	316	38.164	26.691	29.950	1.00	17.08	A
	ATOM	1946	CA	LEU			39.102	26.429	28.854		16.41	A
	ATOM	1947	CB	LEU			38.414	25.636	27.738		13.81	A
30	ATOM	1948	CG	LEU			38.028	24.201	28.115		14.39	A
	ATOM	1949	CD1	LEU		316	37.139	23.597	27.031		12.38	A
	ATOM	1950		LEU			39.302	23.373	28.309		12.77	A
	ATOM	1951	C	LEU			39.652	27.743	28.290		17.12	A
	ATOM	1952	0	LEU			40.851	27.860	28.023		16.53	A
35	ATOM	1953	N	LEU			38.780	28.729	28.105		16.27	A
-	ATOM	1954	CA	LEU			39.228	30.022	27.596		17.52	A
	ATOM	1955	CB	LEU			38.083	30.752	26.887		16.37	A
	ATOM	1956	CG	LEU			37.448	29.973	25.727		18.81	A
	ATOM	1957		LEU			36.415	30.851	25.018		16.47	A
40	ATOM	1958		LEU			38.528	29.526	24.741		17.87	A
40	ATOM	1959	C	LEU			39.745	30.841	28.774		18.27	A
	ATOM	1960	Ö	LEU			39.078	31.753	29.273		18.58	A
	ATOM	1961	N	VAL			40.937	30.475	29.229		18.02	A
	ATOM	1962	CA	VAL			41.593	31.141	30.342		18.85	A
45	ATOM	1963	CB	VAL			41.846	30.153	31.500		19.91	A
43	ATOM	1964		VAL			42.590	30.133	32.634		20.01	A
	ATOM	1965		VAL			40.520	29.584	31.990		19.44	A
	ATOM	1966	C	VAL			42.923	31.657	29.811		19.67	A
50	ATOM	1967	0	VAL			43.690	30.902	29.208		18.26	A
30	ATOM	1968	N	LEU			43.197	32.939	30.028		20.07	A
	MOTA	1969	CA	LEU			44.436	33.533	29.538		20.98	A
	ATOM	1970	CB	LEU			44.521	35.002	29.968		21.64	A
	MOTA	1971	CG	LEU			43.418	35.908	29.408		24.38	A
	MOTA	1972		LEU			43.606	37.332	29.935		23.28	A
55	MOTA	1973		LEU			43.453	35.887	27.875		24.33	A
	MOTA	1974	C	LEU			45.680	32.774	29.994		20.38	A
	MOTA	1975	0	LEU			46.568	32.496	29.192		21.34	A
	MOTA	1976	N	ASP			45.742	32.440	31.280		20.22	A
	MOTA	1977	CA	ASP	A	320	46.879	31.707	31.833	1.00	20.90	A

	ATOM	1978	CB	ASP	Α	320	46.842	31.760	33.365	1.00	20.76	A
	ATOM	1979	CG	ASP	А	320	48.049	31.102	34.004	1.00	21.51	A
	ATOM	1980	OD1	ASP	'n	320	48.669	30.226	33.367	1 00	23.46	A
	MOTA	1981		ASP.		320	48.371	31.450	35.159		23.89	A
5	ATOM	1982	C	ASP	Α	320	46.814	30.247	31.367	1.00	20.06	A
	ATOM	1983	0	ASP	Α	320	45.988	29.476	31.840	1.00	20.54	A
	ATOM	1984	N	ALA.	A	321	47.700	29.876	30.451	1.00	20.68	A
	ATOM	1985	CA	ALA			47.733	28.522	29.903		22.04	A
			CB									
	ATOM	1986		ALA			48.860	28.411	28.881		20.75	A
10	MOTA	1987	C	ALA .			47.858	27.400	30.940		21.62	A
	MOTA	1988	0	ALA	Α	321	47.482	26.259	30.665	1.00	21.99	A
	ATOM	1989	N	THR	Α	322	48.372	27.715	32.127	1.00	20.89	A
	ATOM	1990	CA	THR	А	322	48.531	26.698	33.167	1.00	20.82	A
	ATOM	1991	CB	THR			49.670	27.051	34.146		19.47	A
15				THR			49.341	28.253	34.848		20.19	
13	MOTA	1992										A
	ATOM	1993		THR			50.981	27.249	33.394		21.59	A
	MOTA	1994	С	THR	Α	322	47.264	26.498	33.983	1.00	19.55	A
	ATOM	1995	0	THR	Α	322	47.235	25.673	34.894	1.00	21.13	A
	ATOM	1996	N	LYS	A	323	46.216	27.248	33.661	1.00	19.33	A
20	ATOM	1997	CA	LYS			44.962	27.122	34.392		21.20	A
20	ATOM	1998	CB	LYS			44.580	28.460	35.030		23.75	A
	MOTA	1999	CG	LYS			45.562	28.933	36.084		28.45	A
	ATOM	2000	CD	LYS			45.055	30.177	36.799		33.76	A
	ATOM	2001	CE	LYS	Α	323	46.087	30.678	37.802	1.00	36.15	A
25	ATOM	2002	NZ	LYS	Α	323	46.532	29.569	38.693	1.00	37.34	A
	ATOM	2003	C	LYS			43.806	26.614	33.539	1 00	20.68	A
	ATOM	2004	o	LYS			42.649	26.757	33.915		20.42	A
	MOTA	2005	N	ARG			44.114	26.019	32.392		19.97	A
	MOTA	2006	CA	ARG			43.060	25.494	31.531		17.98	A
30	ATOM	2007	CB	ARG	Α	324	43.461	25.609	30.061	1.00	15.95	A
	ATOM	2008	CG	ARG	Α	324	43.534	27.050	29.603	1.00	17.34	A
	ATOM	2009	CD	ARG			43.996	27.194	28.172	1.00	19.80	A
	ATOM	2010	NE	ARG			44.438	28.565	27.944		16.93	A
	MOTA	2011	CZ	ARG			45.410	28.908	27.108		19.88	A
35	ATOM	2012		ARG			46.045	27.978	26.398		14.58	A
	ATOM	2013	NH2	ARG	Α	324	45.774	30.181	27.015	1.00	16.51	A
	MOTA	2014	C	ARG	Α	324	42.762	24.046	31.883	1.00	18.32	A
	ATOM	2015	0	ARG	Α	324	43.673	23.222	32.006	1.00	18.20	A
	ATOM	2016	N	LEU			41.479	23.748	32.055	1.00	18.32	A
40	ATOM	2017	CA	LEU			41.050	22.403	32.395		17.79	A
40	ATOM	2018	CB	LEU			39.523	22.335	32.425		17.03	A
	MOTA	2019	CG	LEU			38.896	21.125	33.116		15.91	A
	MOTA	2020		LEU			39.392	21.048	34.557		15.93	A
	MOTA	2021	CD2	LEU.	Α	325	37.375	21.255	33.084	1.00	16.56	A
45	ATOM	2022	С	LEU	Α	325	41.599	21.433	31.356	1.00	18.68	A
	ATOM	2023	0	LEU			41.347	21.586	30.157		18.28	A
	ATOM	2024	N	GLY			42.354	20.439	31.821		18.18	A
	MOTA	2025	CA	GLY			42.931	19.462	30.915		16.36	A
	MOTA	2026	C	GLY			44.443	19.558	30.807		19.15	A
50	MOTA	2027	0	GLY	A	326	45.093	18.592	30.404	1.00	19.52	A
	ATOM	2028	N	CYS	Α	327	45.016	20.708	31.161	1.00	18.16	A
	ATOM	2029	CA	CYS			46.463	20.867	31.075		19.30	A
	ATOM	2030	CB	CYS			46.856	22.350	31.058		20.22	A
	MOTA	2031	SG	CYS			46.782	23.200	32.649		21.97	A
55	MOTA	2032	C	CYS			47.169	20.157	32.228		20.22	A
	MOTA	2033	0	CYS	Α	327	46.561	19.828	33.246	1.00	17.92	A
	ATOM	2034	N	GLU	Α	328	48.463	19.933	32.053	1.00	20.51	A
	ATOM	2035	CA	GLU			49.274	19.244	33.042		23.34	A
	ATOM	2036	CB	GLU			50.710	19.139	32.507		28.68	A
	ALOM	2030	CD	GHO	м	320	50.710	10.139	32.307	1.00	20.00	А

	ATOM	2037	CG	GLU	70	229	50.754	18.367	31.175	1.00 38.2	1 A
	ATOM	2039	CD	GLU			52.067	18.500	30.414	1.00 43.2	
	MOTA	2039		GLU			52.535	19.643	30.218	1.00 46.2	
	MOTA	2040		GLU			52.618	17.459	29.991	1.00 44.9	
5	ATOM	2041	C	GLU			49.234	19.876	34.435	1.00 22.1	
	MOTA	2042	0	GLU	Α	328	49.147	19.161	35.437	1.00 20.2	7 A
	ATOM	2043	N	GLU	Α	329	49.276	21.204	34.506	1.00 18.4) A
	ATOM	2044	CA	GLU	Α	329	49.248	21.875	35.801	1.00 20.1	3 A
	ATOM	2045	CB	GLU	Α	329	49.587	23.363	35.657	1.00 20.3	5 A
10	ATOM	2046	CG	GLU	А	329	51.014	23.651	35.190	1.00 24.0	
	ATOM	2047	CD	GLU			51.191	23.518	33.688	1.00 25.9	
	ATOM	2048		GLU			50.213	23.154	32.995	1.00 26.6	
	ATOM	2049		GLU			52.311	23.781	33.198	1.00 27.1	
	ATOM	2050	C	GLU			47.890	21.718	36.480	1.00 19.3	
1.5											
15	MOTA	2051	0	GLU			47.775	21.879	37.694	1.00 18.7	
	ATOM	2052	N	MET			46.863	21.415	35.691	1.00 17.2	
	MOTA	2053	CA	MET			45.520	21.220	36.229	1.00 16.3	
	ATOM	2054	CB	MET			44.474	21.833	35.294	1.00 17.6	
	MOTA	2055	CG	MET			44.460	23.365	35.311	1.00 22.9	
20	ATOM	2056	SD	MET	Α	330	44.186	24.026	36.979	1.00 26.7	3 A
	ATOM	2057	CE	MET	Α	330	42.435	23.712	37.186	1.00 24.6) A
	MOTA	2058	C	MET	Α	330	45.257	19.730	36.422	1.00 14.3) A
	ATOM	2059	0	MET	Α	330	44.127	19.304	36.629	1.00 15.3	9 A
	ATOM	2060	N	GLU	Α	331	46.327	18.949	36.346	1.00 15.6) A
25	ATOM	2061	CA	GLU			46.289	17.501	36.531	1.00 17.0	
	ATOM	2062	CB	GLU			45.607	17.155	37.862	1.00 17.0	
	ATOM	2063	CG	GLU			46.070	18.027	39.038	1.00 17.4	
	ATOM	2064	CD	GLU			47.591	18.179	39.145	1.00 20.1	
	ATOM	2065		GLU			48.034	19.073	39.896	1.00 21.3	
30				GLU							
30	ATOM	2066					48.345	17.420	38.500	1.00 18.8	
	ATOM	2067	C	GLU			45.697	16.658	35.398	1.00 17.8	
	ATOM	2068	0	GLU			45.107	15.602	35.636	1.00 20.4	
	MOTA	2069	N	GLY			45.844	17.133	34.167	1.00 16.2	
	ATOM	2070	CA	GLY			45.420	16.353	33.015	1.00 14.1	
35	ATOM	2071	C	GLY			43.982	16.154	32.596	1.00 13.5	
	ATOM	2072	0	GLY			43.063	16.864	33.017	1.00 11.9	5 A
	MOTA	2073	N	TYR			43.804	15.141	31.750	1.00 14.3	7 A
	MOTA	2074	CA	TYR	Α	333	42.510	14.806	31.182	1.00 13.5	5 A
	ATOM	2075	CB	TYR	Α	333	42.722	13.892	29.968	1.00 15.0	A 0
40	ATOM	2076	CG	TYR	Α	333	43.153	14.683	28.752	1.00 16.4	6 A
	ATOM	2077	CD1	TYR	А	333	42.206	15.172	27.849	1.00 15.2	9 A
	ATOM	2078		TYR			42.573	16,002	26.794	1.00 13.4	
	ATOM	2079	CD2	TYR			44.490	15.039	28.561	1.00 14.9	
	ATOM	2080		TYR			44.872	15.877	27.499	1.00 14.8	
45	ATOM	2081	CZ	TYR			43.902	16.353	26.626	1.00 15.6	
75	ATOM	2082	OH	TYR			44.244	17.197	25.599	1.00 17.2	
	ATOM	2082	C	TYR			41.470	14.230	32.127	1.00 17.2	
	ATOM	2084	0	TYR			40.278	14.323	31.846	1.00 16.6	
	ATOM	2085	N	GLY			41.907	13.650	33.244	1.00 15.5	
50	MOTA	2086	CA	GLY			40.957	13.100	34.202	1.00 15.0	
	ATOM	2087	C	GLY			39.925	14.146	34.616	1.00 16.4	
	MOTA	2088	0	GLY			38.724	13.946	34.433	1.00 15.0	
	MOTA	2089	N	PRO	Α	335	40.366	15.278	35.184	1.00 14.9	5 A
	ATOM	2090	CD	PRO	Α	335	41.727	15.531	35.689	1.00 15.8	3 A
55	MOTA	2091	CA	PRO	Α	335	39.444	16.339	35.606	1.00 15.2) A
	ATOM	2092	CB	PRO	Α	335	40.383	17.397	36.178	1.00 13.1	9 A
	ATOM	2093	CG	PRO			41.485	16.569	36.758	1.00 13.8	
	ATOM	2094	C	PRO			38.594	16.877	34.448	1.00 15.8	
	ATOM	2095	ō	PRO			37.423	17.204	34.631	1.00 14.8	
			-								

	ATOM	2096	N	LEU	Α	336	39.184	16.971	33.257	1.00	16.12	A
	ATOM	2097	CA	LEU	Δ	336	38.450	17.465	32.094		15.52	A
	MOTA	2098	CB	LEU			39.396	17.653	30.898		14.39	A
	MOTA	2099	CG	LEU	Α	336	38.770	17.991	29.538	1.00	15.46	A
5	ATOM	2100	CD1	LEU	Α	336	37.836	19.182	29.662	1.00	11.25	A
	MOTA	2101		LEU			39.884	18.285	28.528		14.11	A
	ATOM	2102	C	LEU			37.321	16.508	31.714		16.28	
												A
	MOTA	2103	0	LEU			36.176	16.921	31.540		15.51	A
	MOTA	2104	N	LYS	Α	337	37.640	15.225	31.592	1.00	17.22	A
10	ATOM	2105	CA	LYS	Α	337	36.624	14.243	31.235	1.00	17.39	A.
	ATOM	2106	CB	LYS	A	337	37.293	12,900	30.921	1.00	17.68	А
	ATOM	2107	CG	LYS			38.170	12.994	29.676		22.31	A
	MOTA	2108	CD	LYS			39.213	11.892	29.592		24.60	A
	MOTA	2109	CE	LYS			38.620	10.560	29.189		24.76	A
15	MOTA	2110	NZ	LYS	Α	337	39.710	9.560	28.997	1.00	25.05	A
	ATOM	2111	C	LYS	Α	337	35.577	14.096	32.342	1.00	17.33	A
	ATOM	2112	0	LYS	Δ	337	34.456	13.652	32.090	1.00	14.42	A
	ATOM	2113	N	ALA			35.928	14.500	33.559		15.83	A
	MOTA	2114	CA	ALA			34.989	14.395	34.674		17.52	A
20	MOTA	2115	CB	ALA	Α	338	35.749	14.167	35.980	1.00	19.68	A
	ATOM	2116	C	ALA	Α	338	34.095	15.621	34.804	1.00	18.83	A.
	ATOM	2117	0	ALA	А	338	33.252	15.687	35.695	1.00	18.94	A
	ATOM	2118	N	HIS			34.262	16.596	33.918		19.42	A
	ATOM	2119	CA	HIS			33.438	17.796	34.004			
											19.28	A
25	MOTA	2120	CB	HIS			33.865	18.819	32.949		19.20	A
	MOTA	2121	CG	HIS	Α	339	33.163	20.134	33.074	1.00	20.26	A.
	ATOM	2122	CD2	HIS	Α	339	33.549	21.299	33.649	1.00	18.95	A
	MOTA	2123	ND1	HIS	А	339	31.880	20.340	32.612	1.00	19.10	A
	ATOM	2124		HIS			31.506	21.576	32.896		22.19	A
20												
30	MOTA	2125		HIS			32.500	22.179	33.525		21.98	A
	MOTA	2126	C	HIS			31.957	17.448	33.845		19.13	A
	MOTA	2127	0	HIS	Α	339	31.597	16.576	33.061	1.00	19.52	A
	ATOM	2128	N	PRO	Α	340	31.079	18.125	34.606	1.00	19.80	A
	MOTA	2129	CD	PRO	Δ	340	31.424	19.119	35.640	1 00	19.08	A
35	ATOM	2130	CA	PRO			29.630	17.900	34.569		20.52	A
33												
	MOTA	2131	CB	PRO		340	29.091	19.058	35.396		20.74	A
	MOTA	2132	CG	PRO			30.146	19.207	36.454		19.20	A
	MOTA	2133	C	PRO	Α	340	29.000	17.834	33.176	1.00	21.42	A
	ATOM	2134	0	PRO	Α	340	28.049	17.088	32.955	1.00	22.48	A
40	ATOM	2135	N	PHE			29.528	18.606	32.237	1.00	21.33	A
	ATOM	2136	CA	PHE			28.985	18.610	30.886		21.57	A
	ATOM	2137	CB	PHE			29.739	19.624	30.017		21.64	A
	MOTA	2138	CG	PHE			29.207	19.740	28.613		23.18	A
	MOTA	2139	CD1	PHE	Α	341	27.903	20.171	28.382	1.00	22.58	A
45	MOTA	2140	CD2	PHE	Α	341	30.013	19.431	27.522	1.00	21.95	A
	ATOM	2141	CE1	PHE	A	341	27.410	20.292	27.082	1.00	23.54	A
	ATOM	2142		PHE			29.533	19.548	26.220		21.83	A
	ATOM	2143	CZ	PHE					25.998		23.23	A
							28.228	19.980				
	MOTA	2144	C	PHE			29.055	17.226	30.237		21.84	A
50	MOTA	2145	0	PHE	Α	341	28.232	16.896	29.389	1.00	20.37	A
	ATOM	2146	N	PHE	Α	342	30.034	16.422	30.640	1.00	20.51	A
	MOTA	2147	CA	PHE	А	342	30.221	15.085	30.077	1.00	23.01	A
	ATOM	2148	СВ	PHE			31.710	14.809	29.850		18.00	A
	MOTA	2149	CG	PHE			32.398	15.812	28.971		17.05	A
55	MOTA	2150		PHE			32.010	15.987	27.652		17.78	A
	MOTA	2151	CD2	PHE	Α	342	33.487	16.534	29.450	1.00	15.72	A
	ATOM	2152	CE1	PHE	Α	342	32.702	16.867	26.811	1.00	18.08	A
	MOTA	2153	CE2	PHE	А	342	34.184	17.414	28.617	1.00	17.45	A
	ATOM	2154	CZ	PHE			33.790	17.578	27.298		16.56	A
	ATOM	2134	CZ	LITE	М	342	33.790	11.370	21.250	1.00	10.50	А

	ATOM	2155	C	PHE A	342	29.679	13.972	30.976	1.00 24.95	A
	ATOM	2156	0	PHE 2	342	30.002	12.798	30.777	1.00 23.95	A
	ATOM	2157		GLU A		28.861	14.333	31.958	1.00 27.35	A
			N							
	MOTA	2158	CA	GLU A		28.325	13.349	32.897	1.00 30.28	A
5	ATOM	2159	CB	GLU A	343	27.187	13.964	33.716	1.00 32.20	A
	ATOM	2160	CG	GLU Z	343	26.581	12.991	34.714	1.00 39.71	A
	ATOM	2161	CD	GLU Z		25.628	13.661	35.688	1.00 44.72	A
	MOTA	2162		GLU A		24.661	14.314	35.234	1.00 47.55	A
	ATOM	2163	OE2	GLU A	343	25.847	13.526	36.911	1.00 46.89	A
10	ATOM	2164	C	GLU A	343	27.852	12.017	32.305	1.00 28.98	A.
	ATOM	2165	o	GLU Z		28.225	10.952	32.800	1.00 31.73	A
	MOTA	2166	N	SER A		27.037	12.067	31.258	1.00 26.09	A
	MOTA	2167	CA	SER A		26.520	10.838	30.656	1.00 28.36	A
	ATOM	2168	CB	SER A	344	25.129	11.089	30.067	1.00 28.73	A.
15	ATOM	2169	OG	SER A	344	25.203	11.942	28.940	1.00 30.91	A
	ATOM	2170	C	SER A		27.407	10.214	29.577	1.00 27.66	A
	MOTA	2171	0	SER A		26.987	9.281	28.900	1.00 28.66	A
	MOTA	2172	N	VAL A		28.627	10.715	29.419	1.00 26.75	A
	MOTA	2173	CA	VAL A	345	29.534	10.183	28.402	1.00 23.44	A
20	ATOM	2174	CB	VAL A	345	30.565	11.256	27.950	1.00 23.10	A
	ATOM	2175	CG1	VAL A		31.589	10.631	26.995	1.00 22.24	A
	ATOM	2176		VAL A		29.854	12.418	27.275	1.00 20.05	A
	MOTA	2177	C	VAL A		30.326	8.957	28.855	1.00 24.26	A
	MOTA	2178	0	VAL A	345	30.876	8.930	29.960	1.00 22.83	A.
25	ATOM	2179	N	THR A	346	30.374	7.942	27.997	1.00 21.77	A.
	ATOM	2180	CA	THR A	346	31.153	6.740	28.272	1.00 23.70	A
	ATOM	2181	CB	THR A		30.391	5.455	27.857	1.00 26.53	A
	MOTA	2182		THR A		29.248	5.284	28.706	1.00 29.98	A
	MOTA	2183	CG2	THR A	346	31.289	4.231	27.990	1.00 24.28	A
30	ATOM	2184	C	THR A	346	32.383	6.945	27.385	1.00 23.43	A.
	MOTA	2185	0	THR A	346	32.306	6.827	26.160	1.00 24.50	A
	ATOM	2186	N	TRP A		33.508	7.270	28.013	1.00 22.98	A
	MOTA	2187	CA	TRP A		34.744	7.569	27.300	1.00 23.81	A
	MOTA	2188	CB	TRP A		35.683	8.352	28.219	1.00 22.54	A
35	MOTA	2189	CG	TRP A	347	35.128	9.658	28.693	1.00 20.61	A
	ATOM	2190	CD2	TRP A	347	35.257	10.927	28.040	1.00 19.11	A
	ATOM	2191		TRP A		34.581	11.881	28.838	1.00 18.39	A
	MOTA	2192		TRP A		35.878	11.351	26.858	1.00 18.16	A
	MOTA	2193		TRP A		34.397	9.883	29.828	1.00 18.35	A
40	MOTA	2194	NE1	TRP A	347	34.065	11.218	29.923	1.00 19.51	A
	ATOM	2195	CZ2	TRP A	347	34.510	13.234	28.491	1.00 16.88	A
	ATOM	2196	CZ3	TRP A	347	35.808	12,701	26.511	1.00 17.23	A
	ATOM	2197		TRP A		35.127	13.624	27.327	1.00 18.16	A
	MOTA	2198	С	TRP A		35.538	6.429	26.675	1.00 25.79	A
45	MOTA	2199	0	TRP A		36.304	6.654	25.742	1.00 24.67	A
	ATOM	2200	N	ALA A	348	35.360	5.215	27.183	1.00 27.10	A
	ATOM	2201	CA	ALA A	348	36.116	4.063	26,697	1.00 27.46	A
	ATOM	2202	CB	ALA A		35.899	2.869	27.636	1.00 27.09	A
	MOTA	2203	C	ALA A		35.895	3.620	25.256	1.00 27.18	A
50	MOTA	2204	0	ALA A	348	36.830	3.148	24.613	1.00 29.41	A
	ATOM	2205	N	ASN A	349	34.682	3.769	24.735	1.00 26.55	A
	ATOM	2206	CA	ASN A	349	34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	СВ	ASN A		33,700	1.962	23.444	1.00 29.37	A
	MOTA	2208	CG	ASN A		32.299	2.088	24.013	1.00 30.92	A
55	MOTA	2209		ASN A		32.045	2.942	24.859	1.00 30.17	A
	ATOM	2210	ND2	ASN A	349	31.386	1.237	23.553	1.00 33.52	A
	MOTA	2211	C	ASN A	349	33.599	4.265	22.509	1.00 26.47	A
	ATOM	2212	ō	ASN A		32.669	3.843	21.819	1.00 25.87	A
	ATOM	2213	N	LEU A		33.947	5.543	22.518	1.00 24.45	A
	ATOM	4413	14	TEO 1		33.941	J. J43	22.318	1.00 24.45	A

	ATOM	2214	CA	TEII	70	350	33.203	6.510	21.721	1.00	22 14	A
	ATOM	2215	CB			350	33.837	7.898	21.848	1.00		A
	ATOM	2216	CG			350	33.659	8.605	23.191	1.00		A
	MOTA	2217	CD1	LEU	Α	350	34.646	9.756	23.293	1.00	19.36	A
5	ATOM	2218	CD2	LEU	А	350	32,220	9.094	23.319	1.00	18.78	A
	ATOM	2219	C			350	33.082	6.152	20.240	1.00		A
	ATOM	2220	ō			350	32.011	6.296	19.650	1.00		A
	MOTA	2221	N	HIS			34.165	5.689	19.627	1.00		A
	MOTA	2222	CA	HIS			34.089	5.387	18.204	1.00		A
10	MOTA	2223	CB	HIS	Α	351	35.506	5.325	17.596	1.00	29.36	A
	ATOM	2224	CG	HIS	Α	351	36.082	3.950	17.493	1.00	32.07	A
	ATOM	2225	CD2	HIS	А	351	36.611	3.128	18.431	1.00	32.39	A
	ATOM	2226	ND1	HIS	Δ	351	36.197	3.285	16.291	1.00		A
	ATOM	2227		HIS			36.775	2.113	16.493	1.00		A
15	ATOM	2228		HIS			37.036	1.992	17.782	1.00		A
13												
	MOTA	2229	C	HIS			33.258	4.144	17.874	1.00		A
	MOTA	2230	0	HIS			33.015	3.847	16.707	1.00		A
	ATOM	2231	N			352	32.800	3.442	18.908	1.00		A
	ATOM	2232	CA	GLN	Α	352	31.963	2.255	18.726	1.00	29.67	A
20	ATOM	2233	CB	GLN	Α	352	32.366	1.145	19.694	1.00	30.56	A.
	ATOM	2234	CG	GLN	А	352	33.169	0.041	19.041	1.00	30.88	A
	ATOM	2235	CD			352	34.493	-0.186	19.729	1.00		A
	ATOM	2236		GLN			34.541	-0.450	20.928	1.00		A
2.5	ATOM	2237		GLN			35.578	-0.084	18.971	1.00		A
25	ATOM	2238	C			352	30.504	2.638	18.963	1.00		A
	ATOM	2239	0			352	29.595	1.831	18.770	1.00		A
	MOTA	2240	N	GLN	Α	353	30.290	3.875	19.397	1.00	27.64	A
	ATOM	2241	CA	GLN	Α	353	28.948	4.365	19.652	1.00	27.42	A
	ATOM	2242	CB	GLN	Α	353	28.977	5.401	20.775	1.00	25.77	A
30	ATOM	2243	CG	GLN.	А	353	29.408	4.837	22.115	1.00	27.34	A
	ATOM	2244	CD			353	29.638	5.914	23.156	1.00		A
	ATOM	2245		GLN			28.875	6.872	23.252	1.00		A
	MOTA	2246		GLN			30.687	5.753	23.951	1.00		A
	MOTA	2247	С			353	28.375	4.989	18.385	1.00		A
35	ATOM	2248	0			353	29.118	5.455	17.516	1.00		A
	ATOM	2249	N	THR	Α	354	27.053	4.984	18.276	1.00	27.31	A
	ATOM	2250	CA	THR	Α	354	26.390	5.568	17.119	1.00	27.85	A
	ATOM	2251	CB	THR	Α	354	24.991	4.941	16.904	1.00	30.69	A
	ATOM	2252	og1	THR	А	354	25.132	3.532	16.665	1.00	30.07	A
40	ATOM	2253		THR			24.289	5.585	15.709	1.00		A
	ATOM	2254	C			354	26.244	7.062	17.376	1.00		A
	ATOM	2255	o			354	25.592	7.475	18.329	1.00		A
	MOTA	2256	N			355	26.867	7.898	16.533	1.00		A
	MOTA	2257	CD			355	27.792	7.588	15.431	1.00		A
45	ATOM	2258	CA			355	26.763	9.346	16.734	1.00	27.23	A
	ATOM	2259	CB	PRO	Α	355	27.625	9.915	15.609	1.00	24.91	A
	ATOM	2260	CG	PRO	Α	355	28.643	8.838	15.385	1.00	25.54	A
	ATOM	2261	C	PRO	А	355	25.322	9.837	16.641	1.00	28.07	A
	ATOM	2262	ō			355	24.548	9.364	15.810	1.00		A
50	ATOM	2263	N			356	24.941	10.792	17.500	1.00		A
50												
	ATOM	2264	CD			356	25.752	11.560	18.462	1.00		A
	MOTA	2265	CA			356	23.572	11.306	17.448	1.00		A
	MOTA	2266	CB			356	23.539	12.301	18.604	1.00		A
	MOTA	2267	CG	PRO	Α	356	24.946	12.832	18.612	1.00	26.86	A
55	MOTA	2268	C	PRO	Α	356	23.363	11.978	16.097	1.00	29.25	A
	ATOM	2269	0	PRO	Α	356	24.304	12.537	15.529	1.00	27.27	A
	ATOM	2270	N	ALA			22.143	11.910	15.575	1.00		A
	ATOM	2271	CA	ALA			21.848	12.521	14.287	1.00		A
	ATOM	2272	CB			357	20.507	12.019	13.757	1.00		A
	AION	4414	CD	мим	м	201	20.307	12.019	13.131	1.00	JI. 79	A

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	ATOM	2273	C	ALA			21.824	14.035	14.448		35.05	A
	MOTA	2274	0	ALA	Α	357	21.194	14.561	15.369	1.00	35.04	A
	MOTA	2275	N	LEU	Α	358	22.516	14.730	13.552	1.00	37.81	A
	ATOM	2276	CA	LEU	Α	358	22.578	16.185	13.597	1.00	42.15	A
5	ATOM	2277	CB	LEU			23.679	16.681	12.658		39.54	A
-	ATOM	2278	CG	LEU			25.086	16.285	13.109		39.51	A
	ATOM	2279		LEU			26.102	16.686	12.062		39.29	A
	MOTA	2280		LEU			25.395	16.953	14.445		40.01	A
	MOTA	2281	C	LEU			21.241	16.837	13.242		45.91	A
10	MOTA	2282	0	LEU			20.874	16.927	12.069		45.71	A
	ATOM	2283	N	THR	Α	359	20.530	17.290	14.275	1.00	50.06	A
	ATOM	2284	CA	THR	Α	359	19.223	17.939	14.140	1.00	53.73	A
	MOTA	2285	CB	THR	Α	359	19.353	19.428	13.726	1.00	54.04	A
	ATOM	2286	og1	THR	А	359	19.995	19.521	12.448	1.00	56.35	A
15	ATOM	2287		THR			20.158	20.204	14.763		54.32	A
	ATOM	2288	C	THR			18.309	17.236	13.139		54.47	A
	ATOM	2289	o	THR			18.483	16.016	12.930		55.90	A
	MOTA	2290		THR			17.407	17.908	12.595		56.97	A
	MOTA	2291	OH2		S	1	42.566	19.118	34.302		15.09	S
20	MOTA	2292	OH2	TIP	S	2	41.052	32.378	19.857		15.82	S
	MOTA	2293	OH2	TIP	S	3	37.014	33.030	17.747	1.00	16.95	S
	MOTA	2294	OH2	TIP	S	5	45.353	24.370	18.152	1.00	16.85	S
	ATOM	2295	OH2	TIP	S	6	31.896	13.930	33.235	1.00	20.42	S
	ATOM	2296	OH2	TIP	s	7	50.351	22.781	28.249	1.00	21.14	s
25	ATOM	2297	OH2	TIP	s	8	45.246	-0.589	-0.734		17.74	S
	ATOM	2298	OH2	TIP	s	11	46.249	-0.348	-8.523		21.32	s
	ATOM	2299	OH2		S	14	45.756	11.148	29.680		21.94	S
	ATOM	2300	OH2	TIP	S	15	44.273	13.157	34.592		15.61	S
	MOTA	2301	OH2	TIP	S	17	53.598	3.722	-1.720		21.45	S
30	MOTA	2302	OH2	TIP	S	18	46.049	13.087	31.565		20.35	S
	MOTA	2303	OH2	TIP	S	19	53.422	22.401	-3.280		23.26	S
	ATOM	2304	OH2	TIP	S	20	34.587	7.922	5.383	1.00	22.58	S
	MOTA	2305	OH2	TIP	S	21	45.053	27.379	19.376	1.00	29.60	S
	ATOM	2306	OH2	TIP	S	23	28.899	36.416	28.633	1.00	31.68	S
35	ATOM	2307	OH2	TIP	s	24	35.531	11.645	-8.219	1.00	23.45	s
	ATOM	2308	OH2	TIP	s	25	47.364	28.787	19.612		23.03	S
	ATOM	2309		TIP	S	27	48.859	21.588	12.634		23.76	S
	ATOM	2310	OH2		S	29	48.805	8.920	23.626		22.23	s
	ATOM	2311		TIP	S	31	48.619	7.247	10.112		21.32	S
40	ATOM	2312		TIP			44.824	28.720	15.621		25.27	S
40					S	34						
	MOTA	2313	OH2		S	35	26.030	12.634	13.407		21.61	S
	MOTA	2314	OH2	TIP	S	36	50.462	19.810	40.066		25.45	S
	ATOM	2315			S	37	39.631	23.510	-0.239		30.88	S
	MOTA	2316	OH2	TIP	S	40	44.734	42.655	10.346	1.00	30.84	S
45	MOTA	2317	OH2	TIP	S	41	54.653	3.902	1.503	1.00	27.14	s
	MOTA	2318	OH2	TIP	S	45	45.693	21.923	39.754	1.00	28.30	S
	ATOM	2319	OH2	TIP	S	47	47.820	16.413	7.805	1.00	25.73	S
	ATOM	2320		TIP	S	48	50.292	31.412	29.642		32.79	S
	ATOM	2321		TIP	S	49	26.056	16.646	34.827		29.80	s
50	ATOM	2322		TIP	s	52	31.714	10.996	31.855		29.15	s
50												
	MOTA	2323	OH2	TIP	S	53	46.108	23.843	-4.299		24.21	S
	MOTA	2324	OH2	TIP	S	54	37.645	11.206	34.448		28.56	S
	ATOM	2325		TIP	S	55	26.371	28.513	12.142		32.08	S
	MOTA	2326		TIP	S	58	33.564	19.700	3.483		28.28	S
55	MOTA	2327	OH2	TIP	S	64	48.295	-0.632	14.280	1.00	32.13	S
	ATOM	2328	OH2	TIP	S	65	40.064	26.036	34.324	1.00	24.17	S
	ATOM	2329	OH2	TIP	S	66	29.570	3.958	14.729	1.00	28.94	S
	ATOM	2330		TIP	S	72	60.085	11.604	6.814		38.35	S
	ATOM	2331		TIP		73	39.203	44.403	18.686		26.61	S
					_	, 5	55.255	- 11 100	_0.000	1.00		2

	3 70037	0220	0770	mrn		20	47 210	10 200	07 266	1 00	00 51	
	MOTA	2332		TIP		76	47.312	12.366	27.366		28.51	S
	MOTA	2333	OH2	TIP	s	80	43.862	33.771	33.329		28.82	S
	MOTA	2334	OH2	TIP	S	81	57.890	13.106	2.128	1.00	40.62	S
	MOTA	2335	OH2	TIP	S	82	41.663	34.381	32.043	1.00	19.35	S
5	ATOM	2336	OH2	TIP	s	8.5	50.974	40.331	19.200	1.00	21.14	S
	MOTA	2337	OH2	TIP	s	88	47.925	-0.832	-6.556		24.11	S
	ATOM	2338	OH2		S	90	27.231	28.336	33.481		27.64	S
	ATOM	2339	OH2		S	91	43.651	-7.101	-7.995		24.33	s
10	MOTA	2340	OH2	TIP	S	92	49.325	4.387	19.370		28.02	S
10	MOTA	2341	OH2		S	93	46.231	11.549	33.898		29.40	S
	MOTA	2342	OH2		S	94	63.889	24.831	1.168		26.53	S
	ATOM	2343	OH2	TIP	S	96	56.396	4.952	-6.749		28.00	S
	MOTA	2344	OH2	TIP	s	98	35.510	27.986	11.558	1.00	29.24	S
	ATOM	2345	OH2	TIP	s	100	49.942	24.366	30.265	1.00	31.61	S
15	ATOM	2346	OH2	TIP	s	101	56.121	7.113	-8.298	1.00	31.57	S
	ATOM	2347	OH2	TIP	s	102	58.318	19.957	-8.378	1.00	26.95	S
	ATOM	2348	OH2			103	49.647	22.446	39.624		40.57	S
	ATOM	2349	OH2		s	104	45.359	7.052	13.052		26.27	S
	ATOM	2350	OH2		s	105	37.150	32.340	32.346		34.45	S
20	ATOM	2351	OH2	TIP	s	107	43.465	40.457	8.240		40.48	S
20		2352				119	36.644	8.257	13.418		30.70	S
	ATOM		OH2									
	MOTA	2353	OH2		S	123	41.912	-8.974	-8.264		26.08	S
	MOTA	2354	OH2		S	124	62.424	15.800	-7.411		24.08	S
	MOTA	2355	OH2	TIP	s	126	37.266	18.656	-9.097	1.00	28.99	S
25	MOTA	2356	OH2		s	127	43.129	26.845	14.606		25.19	S
	ATOM	2357	OH2	TIP	s	128	36.339	32.639	29.802	1.00	29.25	S
	MOTA	2358	OH2	TIP	S	130	54.051	14.561	26.498	1.00	33.93	S
	ATOM	2359	OH2	TIP	S	131	41.805	-4.242	5.492	1.00	33.72	S
	ATOM	2360	OH2	TIP	s	133	38.873	25.163	36.697	1.00	30.69	S
30	ATOM	2361	OH2	TIP	s	134	28.777	8.553	25.307		31.43	S
	ATOM	2362	OH2	TIP	s	135	53.672	10.546	-12.803		33.45	s
	ATOM	2363	OH2	TIP	S	136	59.892	15.434	11.467		31.39	S
	ATOM	2364	OH2			137	31.040	12.361	35.470		34.07	s
	ATOM	2365	OH2		S	139	33.489	14.292	-0.598		40.68	S
2.5												
35	ATOM	2366	OH2		S	140	46.918	8.748	11.662		29.23	S
	MOTA	2367	OH2	TIP	S	141	46.297	-7.287	-9.196		42.20	S
	MOTA	2368	OH2			142	58.193	6.715	-4.685		35.48	S
	MOTA	2369	OH2		S	143	44.598	4.435	12.503		27.68	S
	ATOM	2370			S	144	27.003	5.999	12.450		36.30	S
40	MOTA	2371	OH2	TIP	S	145	43.676	32.852	35.735	1.00	35.70	S
	ATOM	2372	OH2	TIP	S	146	35.783	18.628	36.452	1.00	34.62	S
	MOTA	2373	OH2	TIP	S	147	25.402	4.058	20.638	1.00	45.03	S
	ATOM	2374	OH2	TIP	S	148	45.839	35.853	33.724	1.00	35.47	S
	ATOM	2375	OH2		s	149	22.176	18.976	16.752		31.87	S
45	ATOM	2376	OH2	TIP	s	150	43.986	33.179	10.162	1.00	37.70	s
	ATOM	2377	OH2	TIP	S	151	50.653	20.347	42.428		35.80	s
	ATOM	2378				152	47.843	24.314	9.506		31.05	S
	ATOM	2379			S	153	44.693	5.273	-14.175		29.90	S
			OH2									
50	ATOM	2380				155	26.560	36.851	31.684		49.29	S
50	MOTA	2381	OH2		S	156	46.867		-12.951		29.21	S
	MOTA	2382	OH2			157	30.432	28.741	12.438		37.76	S
	MOTA	2383	OH2		S	158	41.004	20.553	6.423		39.53	S
	MOTA	2384	OH2	TIP	S	159	49.258	20.069	29.294	1.00	33.97	S
	MOTA	2385	OH2	TIP	s	160	48.082	28.459	16.489	1.00	33.10	S
55	MOTA	2386	OH2	TIP	s	161	47.448	18.625	27.683	1.00	34.87	S
	MOTA	2387	OH2	TIP	s	162	19.687	20.632	23.411	1.00	35.01	S
	ATOM	2388	OH2	TIP		163	32.402	-1.266	22.443		37.26	S
	ATOM	2389	OH2			164	39.475	33.468	33.237		35.34	S
	ATOM	2390		TIP			44.277	18.950	5.162		45.14	s
	AIOM	2350	onz	LIP	٥	103	77.2//	10.930	5.162	1.00	40.14	٥

	MOTA	2391	OH2	TIP			34.797	30.523	10.736		47.55	S
	ATOM	2392	OH2	TIP	S	167	46.541	3.526	-14.949	1.00	26.54	S
	ATOM	2393	OH2	TIP	S	168	36.333	16.371	1.539	1.00	38.68	S
	ATOM	2394	OH2		s	169	46.761	38.936	27.403		34.66	S
5												
3	MOTA	2395	OH2		S	170	24.163	13.264	11.375		41.23	S
	MOTA	2396	OH2		s	171	48.459	15.018	31.951		38.11	S
	ATOM	2397	OH2	TIP	S	172	34.261	23.193	40.004	1.00	48.96	S
	ATOM	2398	OH2	TIP	S	173	45.924	-0.026	13.224	1.00	39.55	S
	ATOM	2399	OH2	TIP	g	175	41.384	37.389	32.543	1 00	40.74	S
10	ATOM	2400	OH2	TIP		177	49.394	35.312	27.150		44.33	S
10												
	MOTA	2401	OH2			178	29.066	29.942	34.359		41.46	S
	ATOM	2402	OH2		S	180	49.354	19.467	7.273		34.56	S
	MOTA	2403	OH2	TIP	S	181	25.298	17.029	31.863	1.00	47.74	S
	ATOM	2404	OH2	TIP	S	182	37.071	25.027	4.669	1.00	43.87	S
15	ATOM	2405	OH2	TIP	g	183	22.581	7.487	18.691		41.75	S
	ATOM	2406	OH2		s	184	32.269	7.011	-1.891		48.84	S
	MOTA	2407	OH2	TIP		185	48.234	0.494	6.833		48.16	S
	MOTA	2408	OH2		S	187	20.008	14.658	19.211		45.27	S
	ATOM	2409	OH2	TIP	S	188	49.341	22.698	42.272	1.00	42.20	S
20	ATOM	2410	OH2	TIP	s	190	61.292	18.260	-8.097	1.00	45.21	S
	ATOM	2411	OH2	TIP	s	191	28.152	10.606	2.819		40.38	S
	ATOM	2412	OH2			192	25.626	12.619	23,191		34.27	S
	ATOM	2413	OH2		s	193	59.876	11.603	1.216		46.54	s
	MOTA	2414	OH2		S	194	57.592		-10.646		45.82	S
25	ATOM	2415	OH2		s	195	31.509	36.649	21.499	1.00	38.73	S
	ATOM	2416	OH2	TIP	s	197	50.270	-1.543	-6.136	1.00	42.66	S
	ATOM	2417	OH2	TIP	S	198	24.467	8.729	13.088	1.00	42.78	S
	ATOM	2418	OH2	TIP	S	199	38.098	8.699	25.759	1.00	32.80	s
	ATOM	2419	OH2			200	57.831		-13.255		45.31	S
20												
30	MOTA	2420	OH2		S	201	23.888	22.328	30.524		37.12	S
	MOTA	2421	OH2			202	47.691	26.068	37.666		37.92	S
	ATOM	2422	OH2	TIP	S	203	38.653	7.070	29.307	1.00	50.54	S
	ATOM	2423	OH2	TIP	S	206	44.424	27.583	2.092	1.00	53.50	S
	ATOM	2424	OH2	TIP	S	212	22,258	2.296	17.948	1.00	47.38	s
35	ATOM	2425	OH2	TIP	s	214	19.843	17.943	23.303	1.00	30.36	S
00	ATOM	2426	OH2		S	216	27.647	11.344	24.681		31.32	S
	MOTA	2427	OH2	TIP			37.953	7.817	-9.284		45.97	S
	MOTA	2428	OH2		S	218	33.845	34.040	12.124		38.11	S
	ATOM	2429	OH2	TIP	S	219	58.484	15.269	13.717	1.00	38.26	S
40	ATOM	2430	OH2	TIP	s	220	48.526	40.920	26.583	1.00	35.23	S
	ATOM	2431	OH2	TIP	s	222	52.094	21.184	38.122	1.00	29.86	S
	ATOM	2432	OH2	TIP	S	223	36.889	5.881	3,281	1.00	37.63	s
	ATOM	2433	OH2				47.642		-10.684		34.89	S
		2433		TIP		226			19.133			S
	MOTA		OH2				47.284	2.916			34.10	
45	MOTA	2435	OH2			227	42.468		-15.039		37.98	S
	MOTA	2436	OH2	TIP	s	228	19.169	22.832	21.831	1.00	41.57	S
	ATOM	2437	OH2	TIP	S	231	57.592	12.689	14.880	1.00	50.22	S
	ATOM	2438	OH2	TIP	S	232	27.102	9.176	5.655	1.00	40.57	s
	ATOM	2439	OH2			233	58.618		-11.925		50.71	s
50	ATOM	2440	OH2		S	234	22.822	25.342	19.945		34.93	s
50												
	MOTA	2441	OH2	TIP			24.831	32.218	28.901		37.69	S
	ATOM	2442	OH2	TIP	S	237	20.045	10.774	16.992	1.00	39.57	S
	ATOM	2443	OH2	TIP	S	238	58.019	19.850	15.679	1.00	41.42	S
	ATOM	2444	OH2	TIP	S	239	19.490	20.949	26.114	1.00	34.55	S
55	ATOM	2445		TIP		240	61.187	26.377	7.346		39.68	S
22	ATOM	2446	OH2			241	33.680	38.342	19.389		48.93	S
	MOTA	2447	OH2			242	51.539	31.612	10.881		55.65	S
	MOTA	2448		TIP			25.872	14.431	30.404		46.69	S
	MOTA	2449	OH2	TIP	S	248	37.332	5.849	9.544	1.00	43.81	S

	ATOM	2450		TIP			39.087	-1.293	-9.655		42.96	S
	MOTA	2451	OH2	TIP	S	258	23.938	30.000	30.010	1.00	38.89	S
	ATOM	2452	OH2	TIP	S	259	24.949	29.749	32.578	1.00	40.17	S
	ATOM	2453	OH2	TIP		260	32.111	17.986	1.918		48.36	s
-												
5	MOTA	2454	OH2	TIP		266	21.404	12.876	25.603		57.17	S
	MOTA	2455	OH2	TIP		269	35.425	36.767	12.550	1.00	30.70	S
	ATOM	2456	OH2	TIP	S	270	52.438	25.529	30.131	1.00	44.85	S
	ATOM	2457	OH2	TIP	s	271	53.299	20.156	36.003	1.00	37.15	S
	ATOM	2458	OH2	TIP		272	50.914	6.919	23.723		43.29	s
10		2459					31.578	30.795			50.15	
10	ATOM		OH2	TIP		274			11.014			S
	MOTA	2460	OH2	TIP		275	26.341	7.243	22.447		39.40	S
	ATOM	2461	OH2	TIP	S	276	60.392	18.195	10.235	1.00	37.91	S
	ATOM	2462	OH2	TIP	S	277	47.355	-9.081	-10.821	1.00	48.18	S
	ATOM	2463	OH2	TIP	s	279	41.304	6.175	-16.647	1.00	38.12	S
15	ATOM	2464		TIP		282	33.299	21.620	37.881		46.29	s
13							56.469		-8.575			
	MOTA	2465	OH2	TIP		283		26.112			43.71	S
	MOTA	2466	OH2	TIP		287	48.382	26.573	7.246		41.43	S
	ATOM	2467	OH2	TIP	S	288	56.240	7.245	-11.331	1.00	41.79	S
	MOTA	2468	OH2	TIP	S	290	49.060	14.978	28.166	1.00	37.03	S
20	ATOM	2469	OH2	TIP	s	291	37.095	44.270	26.442	1.00	45.08	S
	ATOM	2470	OH2	TIP		292	47.814		-13.299		48.60	S
	MOTA	2471	OH2			297	58.081	2.784	-7.841		41.89	S
	MOTA	2472		TIP		298	36.447	45.321	18.644		54.91	S
	MOTA	2473	OH2	TIP		299	49.029	23.328	1.767		30.55	S
25	ATOM	2474	OH2	TIP	S	301	24.375	13.771	8.634	1.00	48.47	S
	ATOM	2475	OH2	TIP	S	303	47.904	36.798	28.653	1.00	35.76	S
	ATOM	2476	OH2	TIP	S	305	51.156	40.821	27,172	1.00	43.59	s
	ATOM	2477	OH2	TIP	S	306	32.943	28.917	35.227		42.60	s
	ATOM	2478		TIP	S	307	58.462	28.373	6.251		46.15	s
20			OH2									
30	MOTA	2479	OH2	TIP	S	308	41.964	30.940	36.712		48.26	S
	ATOM	2480	OH2	TIP	S	313	51.176	-1.922	-3.336	1.00	50.61	S
	ATOM	2481	OH2	TIP	SI	.001	21.319	36.868	23.805	1.00	36.97	S
	ATOM	2482	OH2	TIP	SI	.002	48.880	32,620	27.617	1.00	44.40	S
	ATOM	2483	OH2	TIP	S 1	003	61.880	19.473	11.767	1 00	45.49	s
35	ATOM	2484		TIP			52.770	21.424	26.815		24.43	s
33												
	MOTA	2485	OH2	TIP		.005	35.373	29.094	36.197		35.97	S
	MOTA	2486		TIP			40.815	-6.636	4.389		43.15	S
	MOTA	2487	OH2	TIP	SI	.007	44.953	1.286	11.272	1.00	49.45	S
	MOTA	2488	OH2	TIP	SI	.010	21.004	16.168	27.009	1.00	48.51	S
40	ATOM	2489	OH2	TIP	SI	.011	47.094	41.786	9.243	1.00	50.10	S
	ATOM	2490	OH2	TIP	S1	012	32.479	2.978	14.158	1.00	49.47	S
	ATOM	2491		GLC		1	48.557		-12,279		40.72	G
						1			-11.097			
	MOTA	2492		GLC			48.836				38.05	G
	MOTA	2493		GLC		1	49.266		-11.476		38.09	G
45	ATOM	2494		GLC		1	49.559		-10.292	1.00	33.99	G
	MOTA	2495	C15	GLC	G	1	48.150	14.257	-12.257	1.00	37.32	G
	ATOM	2496	016	GLC	G	1	48.574	15.582	-12.604	1.00	36.74	G
	ATOM	2497			G	2	40.114	-6.634	-6.562		33.52	G
	ATOM	2498		GLC		2	38.967	-6.592	-7.404		31.05	G
50						2						
30	MOTA	2499		GLC			37.712	-6.417	-6.552		31.56	G
	MOTA	2500		GLC		2	36.554	-6.406	-7.389		30.70	G
	MOTA	2501	C15	GLC	G	2	37.792	-5.109	-5.761	1.00	30.03	G
	ATOM	2502	016	GLC	G	2	36.609	-4.961	-4.975	1.00	29.66	G
	ATOM	2503		GLC		3	44.030		-13.470		37.90	G
55	ATOM	2504		GLC		3	43.950		-13.690		38.47	G
55												
	MOTA	2505			G	3	42.747		-14.579		39.52	G
	MOTA	2506			G	3	41.551		-13.942		39.39	G
	MOTA	2507		GLC		3	42.878		-15.934		41.43	G
	MOTA	2508	016	GLC	G	3	41.736	9.613	-16.731	1.00	40.78	G

	ATOM	2509	012	GLC	G	5	4	0.556	1.005	2.289	1.00	45.25	G
	ATOM	2510	C11	GLC	G	5	4	0.966	2.332	1.960	1.00	40.56	G
	ATOM	2511			G	5		0.187	3.327	2.814		40.36	G
	ATOM	2512			G	5		88.791	3.169	2.572		40.71	G
5	ATOM	2513		GLC		5		0.619	4.751	2.464		40.04	G
-	ATOM	2514		GLC		5		9.885	5.681	3.256		36.89	G
	ATOM	2515			G	6		6.951	22,702	40.046		63.04	G
	ATOM	2516			G	6		37.592	21.583	39.422		62.46	G
	ATOM	2517		GLC		6		88.104	21.978	38.030		61.14	G
10													
10	MOTA	2518		GLC		6		39.034	23.054	38.168		61.72	G
	ATOM	2519		GLC	G	6		6.948	22.429	37.126		60.51	G
	ATOM	2520			G	6		35.992	21.372	36.960		58.61	G
	MOTA	2521		GLC	G	7		37.316	0.281	14.299		73.45	G
	ATOM	2522		GLC		7		37.655	-0.758	15.222		72.78	G
15	MOTA	2523		GLC	G	7		36.592	-1.856	15.157		72.98	G
	MOTA	2524			G	7		35.320	-1.299	15.498		73.88	G
	ATOM	2525		GLC	G	7	3	36.924	-2.989	16.134		73.66	G
	MOTA	2526			G	7	3	36.972	-2.493	17.478	1.00	75.38	G
	MOTA	2527	012	GLC	G	8	5	1.921	21.898	5.908	1.00	62.51	G
20	ATOM	2528	C11	GLC	G	8	5	2.447	20.871	5.063	1.00	63.42	G
	ATOM	2529	C13	GLC	G	8	5	1.476	20.597	3.908	1.00	64.28	G
	ATOM	2530	014	GLC	G	8	5	1.297	21.794	3.150	1.00	66.28	G
	ATOM	2531	C15	GLC	G	8	5	0.121	20.137	4.448	1.00	64.49	G
	ATOM	2532	016	GLC	G	8	4	9.233	19.886	3.357	1.00	64.01	G
25	ATOM	2533		GLC		10		86.044	37.499	29.523		56.89	G
	ATOM	2534		GLC		10		35.164	36.645	30.259		56.97	G
	ATOM	2535		GLC		10		3.849	36.489	29.494		56.11	G
	ATOM	2536		GLC		10		3.248	37.772	29.308		56.44	G
	ATOM	2537		GLC		10		32.900	35.580	30.277		55.84	G
30	ATOM	2538			G	10		31.674	35.442	29.557		55.39	G
50	ATOM	2539		ATP		1		6.280	25.658	5.170		51.49	N
	ATOM	2540	PG	ATP		1		16.464	25.053	3.691		52.22	N
	ATOM	2541		ATP		1		17.406	23.911	3.763		51.41	N
	ATOM	2542		ATP	N	1		16.794	26.182	2.784		52.07	N
35		2543		ATP				14.976	24.513	3.344		51.01	
33	ATOM				N	1		4.560					N
	ATOM	2544	PB	ATP	N	1			22.969	3.605		50.20	N
	ATOM	2545		ATP		1		13.083	22.898	3.669		49.41	N
	ATOM	2546		ATP	N	1		15.345	22.474	4.766		50.34	N
	ATOM	2547		ATP	N	1		15.070	22.231	2.255		47.77	N
40	ATOM	2548	PA	ATP	N	1		15.075	20.613	2.121		42.84	N
	MOTA	2549		ATP	N	1		15.547	20.291	0.754		43.81	N
	MOTA	2550		ATP	N	1		15.807	20.035	3.270		45.03	N
	MOTA	2551			N	1		3.516	20.223	2.245		41.73	N
	MOTA	2552		ATP		1		12.528	20.925	1.489		37.57	N
45	ATOM	2553	C4*	ATP	N	1	4	11.127	20.379	1.776	1.00	39.45	N
	MOTA	2554	04*	ATP	N	1	4	10.907	19.024	1.279	1.00	37.72	N
	MOTA	2555	C3*	ATP	N	1	4	10.777	20.321	3.251	1.00	38.48	N
	ATOM	2556	03*	ATP	Ν	1	4	10.360	21.615	3.697	1.00	40.42	N
	ATOM	2557	C2*	ATP	N	1	3	9.608	19.374	3.270	1.00	37.58	N
50	MOTA	2558	02*	ATP	N	1	3	88.410	20.076	2.924	1.00	35.98	N
	ATOM	2559	C1*	ATP	N	1	3	9.939	18.346	2.173	1.00	35.55	N
	MOTA	2560	N9	ATP	N	1		0.628	17.156	2.747	1.00	31.76	N
	ATOM	2561	C8		N	1		11.864	17.126	3.274		30.49	N
	ATOM	2562	N7	ATP		1		2.143	15.877	3.667		29.75	N
55	ATOM	2563	C5	ATP	N	1		11.088	15.118	3.390		27.49	N
	ATOM	2564	C4	ATP		1		0.125	15.925	2.810		30.02	N
	ATOM	2565	N3	ATP	N	1		88.937	15.389	2.431		27.11	N
	ATOM	2566	C2	ATP		1		88.679	14.085	2.615		25.62	N
	ATOM	2567	N1	ATP		1		39.597	13.283	3.175		21.76	N

	ATOM	2568	C6	ATP	N	1	40.800	13.768	3.571	1.00	23.90	N
	ATOM	2569	N6	ATP	N	1	41.698	12.964	4.127	1.00	21.94	N
	ATOM	2570	S	SO4	I	1	58.680	8.493	-0.639	1.00	56.05	I
	ATOM	2571	01	SO4	Ι	1	57.956	7.875	0.483	1.00	58.83	I
5	MOTA	2572	02	SO4	Ι	1	57.886	9.607	-1.188	1.00	57.04	I
	MOTA	2573	03	SO4	I	1	58.906	7.478	-1.683	1.00	57.47	I
	ATOM	2574	04	SO4	Ι	1	59.976	9.008	-0.156	1.00	57.51	I
	ATOM	2575	S	SO4	I	2	39.339	4.855	7.057	1.00	84.24	I
	MOTA	2576	01	SO4	I	2	39.390	6.175	7.711	1.00	85.02	I
10	MOTA	2577	02	SO4	I	2	40.101	4.897	5.797	1.00	84.75	I
	ATOM	2578	03	SO4	Ι	2	37.936	4.506	6.766	1.00	84.94	I
	MOTA	2579	04	SO4	Ι	2	39.931	3.842	7.954	1.00	84.44	I
	MOTA	2580	S	SO4	I	3	38.987	-2.256	3.310	1.00	58.58	I
	MOTA	2581	01	SO4	I	3	37.734	-1.675	3.827	1.00	59.11	I
15	MOTA	2582	02	SO4	I	3	39.460	-1.454	2.172		59.91	I
	MOTA	2583	03	SO4	I	3	38.743	-3.640	2.866	1.00	60.97	I
	MOTA	2584	04	SO4	I	3	40.014	-2.260	4.369	1.00		I
	MOTA	2585	S	SO4	I	4	34.397	5.289	30.981		64.34	I
	MOTA	2586	01	SO4	I	4	33.627	6.528	30.742	1.00		I
20	MOTA	2587	02		I	4	34.337	4.427	29.782		60.11	I
	MOTA	2588	03	SO4	I	4	33.816	4.572	32.133		64.39	I
	MOTA	2589	04	SO4	I	4	35.806	5.626	31.277		63.55	I
	MOTA	2590	S	SO4	I	5	55.074	-6.984	-3.711		75.40	I
	MOTA	2591	01		I	5	54.657	-7.518	-2.399	1.00		I
25	MOTA	2592	02	SO4	I	5	54.209	-5.845	-4.065	1.00		I
	MOTA	2593	03	SO4	I	5	54.950	-8.034	-4.742		74.22	I
	MOTA	2594	04	SO4	Ι	5	56.477	-6.532	-3.633		75.15	I
	MOTA	2595	02	PO4	Ρ	100	57.362	24.998	13.149	1.00		P
	MOTA	2596	03	PO4	P	100	59.399	26.166	13.761	1.00		P
30	MOTA	2597	04	PO4	P	100	57.761	25.606	15.462		67.43	P
	MOTA	2598	01	PO4		100	57.264	27.325	13.818	1.00		P
	MOTA	2599	P	PO4	P	100	57.947	26.025	14.048	1.00	66.69	P
	END											

Example 4: Co-ordinates for the dimer of the PDK1 fragment, without alternate side chains. Chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

	MOTA	1	CB	PRO A	71	58.912	-7.251	8.216	1.00 67.78	A
40	ATOM	2	CG	PRO A	71	59.621	-6.941	9.534	1.00 69.16	A
	ATOM	3	С	PRO A	71	59.493	-6.506	5.894	1.00 67.06	A
	ATOM	4	0	PRO A	71	59.196	-5.318	5.766	1.00 66.66	A
	ATOM	5	N	PRO A	71	60.984	-6.073	7.833	1.00 67.86	A
	ATOM	6	CD	PRO A	71	60.554	-5.762	9.207	1.00 68.24	A
45	ATOM	7	CA	PRO A	71	60.040	-7.035	7.217	1.00 67.75	A
	ATOM	8	N	PRO A	72	59.356	-7.385	4.890	1.00 66.32	A
	MOTA	9	CD	PRO A	72	59.712	-8.816	4.898	1.00 67.17	A
	ATOM	10	CA	PRO A	72	58.840	-6.986	3.578	1.00 65.61	A
	MOTA	11	CB	PRO A	72	58.672	-8.321	2.858	1.00 66.47	A
50	ATOM	12	CG	PRO A	72	59.796	-9.133	3.419	1.00 67.57	A
	ATOM	13	C	PRO A	72	57.527	-6.208	3.673	1.00 63.94	A
	ATOM	14	0	PRO A	72	56.710	-6.451	4.561	1.00 64.11	A
	ATOM	15	N	ALA A	73	57.341	-5.268	2.753	1.00 61.57	A
	ATOM	16	CA	ALA A	73	56.133	-4.454	2.708	1.00 58.74	A
55	ATOM	17	CB	ALA A	73	56.438	-3.030	3.165	1.00 58.05	A

	ATOM	18	C	ALA	Α	73	55.626	-4.448	1.271	1.00		A
	MOTA	19	0	ALA		73	56.347	-4.834	0.349	1.00		A
	MOTA	20	N	PRO		74	54.372	-4.024	1.057	1.00		A
	MOTA	21	CD	PRO	A	74	53.335	-3.610	2.018	1.00	53.31	A
5	ATOM	22	CA	PRO	Α	74	53.856	-4.003	-0.314	1.00	52.54	A
	MOTA	23	CB	PRO	A	74	52.474	-3.375	-0.148	1.00	52.86	A
	ATOM	24	CG	PRO	A	74	52.067	-3.824	1.226	1.00	52.88	A
	MOTA	25	C	PRO	A	74	54.772	-3.167	-1.204	1.00	50.08	A
	MOTA	26	0	PRO	A	74	55.559	-2.361	-0.708	1.00	49.96	A
10	MOTA	27	N	ALA	Α	75	54.680	-3.366	-2.514	1.00	47.58	A
	MOTA	28	CA	ALA	A	75	55.503	-2.602	-3.446	1.00	44.69	A
	ATOM	29	CB	ALA	A	75	55.312	-3.121	-4.870	1.00	46.14	A
	MOTA	30	C	ALA	A	75	55.100	-1.134	-3.371	1.00	41.55	A
	ATOM	31	0	ALA	A	75	53.947	-0.813	-3.086	1.00	41.01	A
15	ATOM	32	N	LYS	Α	76	56.053	-0.245	-3.619	1.00	38.31	A
	ATOM	33	CA	LYS	A	76	55.781	1.184	-3.588	1.00	35.72	A
	MOTA	34	CB	LYS	A	76	57.053	1.957	-3.930	1.00	37.70	A
	ATOM	35	CG	LYS	A	76	57.123	3.356	-3.350	1.00	40.99	A
	ATOM	36	CD	LYS	A	76	57.262	3.316	-1.836	1.00	40.04	A
20	ATOM	37	CE	LYS	A	76	57.511	4.705	-1.277	1.00	42.08	A
	ATOM	38	NZ	LYS	Α	76	57.681	4.695	0.202	1.00	42.99	A
	MOTA	39	C	LYS	A	76	54.708	1.467	-4.638	1.00	32.65	A
	ATOM	40	0	LYS	Α	76	54.814	1.005	-5.770	1.00	31.41	A
	ATOM	41	N	LYS	Α	77	53.668	2.207	-4.270	1.00	28.59	A
25	ATOM	42	CA	LYS	A	77	52.619	2.517	-5.232	1.00	25.72	A
	MOTA	43	CB	LYS	Α	77	51.316	2.865	-4.509	1.00	26.22	A
	MOTA	44	CG	LYS	A	77	50.796	1.731	-3.631	1.00	27.15	A
	MOTA	45	CD	LYS	A	77	49.487	2.089	-2.967	1.00	26.80	A
	MOTA	46	CE	LYS	A	77	49.136	1.091	-1.870	1.00	27.31	A
30	MOTA	47	NZ	LYS	A	77	48.998	-0.296	-2.380	1.00	27.17	A
	MOTA	48	C	LYS	A	77	53.053	3.668	-6.137	1.00	24.67	A
	MOTA	49	0	LYS	Α	77	54.010	4.377	-5.829	1.00	21.60	A
	MOTA	50	N	ARG	A	78	52.351	3.838	-7.254	1.00	23.66	A
	ATOM	51	CA	ARG	A	78	52.662	4.897	-8.211	1.00	26.14	A
35	MOTA	52	CB	ARG	A	78	53.574	4.344	-9.318	1.00	28.57	A
	ATOM	53	CG	ARG	A	78	53.017	3.139	-10.050	1.00	34.78	A
	MOTA	54	CD	ARG	A	78	54.092	2.465	-10.896	1.00	40.96	A
	MOTA	55	NE	ARG	A	78	53.560	1.364	-11.700	1.00	48.93	A
	MOTA	56	CZ	ARG	A	78	52.985	0.270	-11.203	1.00	52.58	A
40	ATOM	57	NH1	ARG	A	78	52.860	0.113	-9.889	1.00	54.60	A
	MOTA	58	NH2	ARG	A	78	52.530	-0.672	-12.022	1.00	54.09	A
	MOTA	59	С	ARG	A	78	51.382	5.488	-8.803	1.00	23.76	A
	ATOM	60	0	ARG	A	78	50.311	4.888	-8.706	1.00	24.25	A
	MOTA	61	N	PRO	A	79	51.475	6.676	-9.428	1.00	21.76	A
45	MOTA	62	CD	PRO	Α	79	52.691	7.475	-9.668	1.00	20.82	A
	MOTA	63	CA	PRO	A	79	50.301	7.325	-10.021	1.00	21.96	A
	ATOM	64	CB	PRO	Α	79	50.910	8.481	-10.816	1.00	22.27	A
	MOTA	65	CG	PRO	A	79	52.124	8.831	-10.014	1.00	22.12	A
	MOTA	66	C	PRO	A	79	49.446	6.413	-10.903	1.00	22.86	A
50	MOTA	67	0	PRO	Α	79	48.213	6.461	-10.842	1.00	20.52	A
	ATOM	68	N	GLU	Α	80	50.103	5.586	-11.714	1.00	21.87	A
	MOTA	69	CA	GLU	Α	80	49.403	4.685	-12.628	1.00	22.99	A
	MOTA	70	CB	GLU	A	80	50.393	3.994	-13.571	1.00	25.24	A
	MOTA	71	CG		Α	80	51.230		-12.925	1.00		A
55	MOTA	72	CD	GLU		80	52.157		-13.913	1.00		A
	MOTA	73		GLU		80	53.072		-14.433	1.00		A
	MOTA	74	OE2	GLU	Α	80	51.969	1.015	-14.172	1.00	32.83	A
	MOTA	75	C	GLU		80	48.556		-11.912	1.00		A
	MOTA	76	0	GLU	Α	80	47.692	3.013	-12.530	1.00	22.37	A

	ATOM	77	N	ASP	А	81	48.804	3,413	-10.622	1.00 19.97	A
	ATOM	78	CA	ASP		81	48.026	2.423	-9.874	1.00 19.93	A
	ATOM	79	CB	ASP		81	48.736	2.029	-8.571	1.00 21.19	A
	ATOM	80	CG	ASP		81	50.089	1.380	-8.807	1.00 22.46	A
5	ATOM	81		ASP		81	50.195	0.554	-9.731	1.00 24.22	A
-	ATOM	82		ASP		81	51.043	1.685	-8.058	1.00 23.33	A
	ATOM	83	C	ASP		81	46.652	2.975	-9.518	1.00 20.85	A
	ATOM	84		ASP		81	45.793	2.246	-9.015	1.00 20.05	A
			0								
10	ATOM	85	N	PHE		82	46.445	4.258	-9.804	1.00 18.91	A
10	MOTA	86	CA	PHE		82	45.200	4.934	-9.465	1.00 19.30	A
	MOTA	87	CB			82	45.475	6.027	-8.427	1.00 18.43	A
	MOTA	88	CG	PHE		82	46.134	5.531	-7.175	1.00 18.01	A
	MOTA	89		PHE		82	45.371	5.136	-6.084	1.00 17.19	A
	MOTA	90	CD2	PHE		82	47.520	5.460	-7.086	1.00 18.99	A
15	MOTA	91	CE1	PHE	A	82	45.977	4.676	-4.918	1.00 17.12	A
	MOTA	92	CE2	PHE		82	48.137	5.000	-5.925	1.00 19.64	A
	MOTA	93	CZ	PHE	Α	82	47.361	4.607	-4.838	1.00 18.00	A
	MOTA	94	C	PHE	Α	82	44.476	5.596	-10.621	1.00 20.81	A
	ATOM	95	0	PHE	Α	82	45.066	5.933	-11.649	1.00 20.34	A
20	ATOM	96	N	LYS	Α	83	43.182	5.792	-10.411	1.00 19.80	A
	ATOM	97	CA	LYS	Α	83	42.321	6.478	-11.353	1.00 21.65	A
	MOTA	98	CB	LYS	Α	83	41.096	5.625	-11.687	1.00 22.02	A
	ATOM	99	CG	LYS	Α	83	40.062	6.326	-12.550	1.00 28.93	A
	ATOM	100	CD	LYS		83	38.974		-12.981	1.00 34.20	A
25	ATOM	101	CE	LYS		8.3	37.909		-13.824	1.00 38.10	A
	ATOM	102	NZ	LYS		83	37.179		-13.043	1.00 43.33	A
	ATOM	103	c	LYS		83	41.913		-10.541	1.00 20.74	A
	ATOM	104	ō	LYS		83	41.084	7.606	-9.635	1.00 20.98	A
	ATOM	105	N	PHE		84	42.513		-10.835	1.00 19.99	A
30	ATOM	106	CA			84	42.188		-10.083	1.00 18.63	A
50	ATOM	107	CB	PHE		84	43.279		-10.003	1.00 18.95	A
	ATOM	107	CG	PHE		84	44.571	10.741	-9.587	1.00 17.68	A
	ATOM	108		PHE		84	45.498		-10.224	1.00 17.66	A A
2.5	ATOM	110	CD2	PHE		84	44.843	11.183	-8.299	1.00 19.66	A
35	ATOM	111	CE1			84	46.676	9.556	-9.589	1.00 18.09	A
	ATOM	112	CE2	PHE		84	46.021	10.816	-7.653	1.00 18.89	A
	MOTA	113	CZ	PHE		84	46.936	10.002	-8.301	1.00 17.33	A
	MOTA	114	С	PHE		84	40.834	10.617	-10.460	1.00 19.69	A
	MOTA	115	0	PHE		84	40.391		-11.601	1.00 20.72	A
40	MOTA	116	N	GLY		85	40.178	11.233	-9.484	1.00 16.80	A
	MOTA	117	CA	GLY		85	38.872	11.810	-9.716	1.00 17.73	A
	MOTA	118	C	GLY		85	38.819	13.280	-9.346	1.00 18.75	A
	ATOM	119	0	GLY	A	85	39.740	14.043	-9.650	1.00 18.45	A
	MOTA	120	N	LYS	A	86	37.753	13.673	-8.659	1.00 16.00	A
45	MOTA	121	CA	LYS	A	86	37.571	15.064	-8.278	1.00 18.26	A
	ATOM	122	CB	LYS	A	86	36.133	15.302	-7.812	1.00 19.00	A
	MOTA	123	CG	LYS	A	86	35.793	14.660	-6.481	1.00 21.55	A
	MOTA	124	CD	LYS	A	86	34.368	14.981	-6.066	1.00 26.48	A
	MOTA	125	CE	LYS	Α	86	33.994	14.239	-4.793	1.00 31.92	A
50	ATOM	126	NZ	LYS		86	32.568	14.457	-4.412	1.00 35.36	A
	ATOM	127	C	LYS		86	38.523	15.571	-7.202	1.00 18.57	A
	ATOM	128	ō	LYS		86	39.045	14.807	-6.385	1.00 16.77	A
	ATOM	129	N	ILE		87	38.737	16.881	-7.227	1.00 17.88	A
	ATOM	130	CA	ILE		87	39.577	17.554	-6.256	1.00 18.26	A
55	ATOM	131	CB	ILE		87	39.994	18.952	-6.772	1.00 19.60	A
22	ATOM	132	CG2	ILE		87	40.593	19.786	-5.628	1.00 18.73	A
	ATOM	133	CG1			87	40.393	18.786	-7.945	1.00 18.73	A
	ATOM	134		ILE		87	41.412	20.087	-8.588	1.00 25.26	A
		134	CDI	ILE		87				1.00 25.26	A A
	ATOM	133	U	TPR	А	8 /	38.731	17.709	-4.997	1.00 19.6/	A

	ATOM	136	0	ILE	Δ	87	37.628	18.249	-5.052	1.00 20.41	A
	ATOM	137	N	LEU		88	39.240	17.229	-3.867	1.00 19.15	A
	ATOM	138	CA	LEU		88	38.508	17.324	-2.611	1.00 20.68	A
			CB			88					
-	ATOM	139		LEU			38.870	16.151	-1.700	1.00 19.97	A
5	MOTA	140	CG		A	88	38.529	14.759	-2.237	1.00 19.24	A
	MOTA	141		LEU		88	39.090	13.692	-1.311	1.00 21.41	A
	MOTA	142		LEU		88	37.029	14.622	-2.359	1.00 18.84	A
	ATOM	143	C	LEU		88	38.815	18.632	-1.901	1.00 23.11	A
	MOTA	144	0	LEU		88	37.999	19.146	-1.139	1.00 25.10	A.
10	MOTA	145	N	GLY	Α	89	39.997	19.174	-2.149	1.00 24.09	A
	ATOM	146	CA	GLY	A	89	40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	C	GLY	A	89	41.658	20.954	-2.078	1.00 25.47	A
	ATOM	148	0	GLY	A	89	42.445	20.202	-2.666	1.00 22.19	A
	ATOM	149	N	GLU	Α	90	41.870	22.254	-1.906	1.00 26.22	A
15	ATOM	150	CA	GLU	A	90	43.064	22.924	-2.404	1.00 29.96	A
	ATOM	151	CB	GLU	А	90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU	А	90	42,267	23.038	-4.831	1.00 34.32	A
	ATOM	153	CD	GLU		90	41.711	23.930	-5.927	1.00 38.27	A
	ATOM	154		GLU		90	40.590	24.456	-5.764	1.00 40.57	A
20	ATOM	155	OE2			90	42.398	24.110	-6.952	1.00 40.90	A
20	ATOM	156	C	GLU		90	43.711	23.768	-1.313	1.00 30.68	A
	ATOM	157	o	GLU		90	43.049	24.574	-0.668	1.00 32.83	A
	ATOM	158	N	GLY		91	45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY		91	45.724	24.332	-0.104	1.00 29.40	A
25									-0.798	1.00 29.98	
23	ATOM	160	C	GLY		91	46.795	25.151			A
	ATOM	161	0	GLY		91	46.894	25.130	-2.028	1.00 28.16	A
	MOTA	162	N	SER		92	47.605	25.870	-0.029	1.00 28.30	A
	MOTA	163	CA	SER		92	48.653	26.681	-0.633	1.00 30.50	A
	MOTA	164	CB	SER		92	49.165	27.717	0.370	1.00 32.43	A
30	MOTA	165	OG	SER		92	49.520	27.099	1.593	1.00 40.94	A
	MOTA	166	C	SER		92	49.815	25.843	-1.164	1.00 29.77	A
	ATOM	167	0	SER		92	50.456	26.221	-2.143	1.00 30.46	A
	ATOM	168	N	PHE		93	50.087	24.703	-0.536	1.00 27.65	A
	MOTA	169	CA	PHE	A	93	51.185	23.855	-0.995	1.00 26.34	A
35	ATOM	170	CB	PHE	Α	93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	A	93	52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE	A	93	52.283	25.909	1.392	1.00 29.96	A
	ATOM	173	CD2	PHE	A	93	53.949	25.613	-0.308	1.00 31.38	A
	ATOM	174	CE1	PHE	A	93	52.779	27.181	1.665	1.00 32.69	A
40	ATOM	175	CE2	PHE	A	93	54.452	26.883	-0.044	1.00 32.63	A
	ATOM	176	CZ	PHE	А	93	53.864	27.670	0.945	1.00 31.81	A
	ATOM	177	С	PHE	A	93	50.759	22.445	-1.365	1.00 25.39	A
	ATOM	178	0	PHE	A	93	51.601	21.559	-1.522	1.00 24.59	A
	ATOM	179	N	SER		94	49.457	22.235	-1.519	1.00 23.63	A
45	ATOM	180	CA	SER		94	48.965	20.912	-1.860	1.00 21.43	A
	ATOM	181	CB	SER		94	49.017	20.013	-0.628	1.00 21.42	A
	ATOM	182	OG	SER		94	48.091	20.475	0.340	1.00 21.12	A
	ATOM	183	c	SER		94	47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	0	SER		94	46.795	21.882	-2.173	1.00 19.02	A
50	ATOM	185	N	THR		95	47.174	19.832	-3.038	1.00 19.38	A
50						95			-3.580	1.00 17.98	
	ATOM	186	CA	THR			45.840	19.637			A
	ATOM	187	CB	THR		95	45.818	19.818	-5.110	1.00 19.25	A
	MOTA	188		THR		95	46.196	21.162	-5.434	1.00 22.04	A
	ATOM	189		THR		95	44.421	19.549	-5.661	1.00 17.61	A
55	MOTA	190	С	THR		95	45.455	18.201	-3.243	1.00 18.61	A
	MOTA	191	0	THR		95	46.212	17.264	-3.524	1.00 17.10	A
	MOTA	192	N	VAL		96	44.295	18.024	-2.623	1.00 16.53	A
	ATOM	193	CA	VAL		96	43.845	16.685	-2.266	1.00 16.05	A
	MOTA	194	CB	VAL	Α	96	43.170	16.672	-0.886	1.00 16.32	A

	ATOM	195	CG1	VAL	Α	96	42.741	15.249	-0.532	1.00 18.	02 A
	ATOM	196		VAL		96	44.145	17.206	0.168	1.00 16.	
	ATOM	197	С	VAL		96	42.875	16.207	-3.335	1.00 16.	
	ATOM	198	ō	VAL		96	41.906	16.892	-3.665	1.00 16.	
5	ATOM	199	N	VAL		97	43.157	15.033	-3.888	1.00 16.	
	ATOM	200	CA	VAL		97	42.338	14.471	-4.949	1.00 16.	
	ATOM	201	CB	VAL		97	43.153	14.354	-6.255	1.00 18.	
	ATOM	202		VAL		97	42.249	13.927	-7.404	1.00 19.	
	ATOM	203		VAL		97	43.831	15.685	-6.569	1.00 17.	
10	ATOM	203	C	VAL		97	41.812	13.091	-4.583	1.00 17.	
10											
	ATOM	205	0	VAL		97	42.532	12.270	-4.014	1.00 17.	
	ATOM	206	N	LEU		98	40.545	12.845	-4.895	1.00 16.	
	ATOM	207	CA	LEU		98	39.947	11.548	-4.624	1.00 17.	
	ATOM	208	CB	LEU		98	38.424	11.633	-4.743	1.00 16.	
15	MOTA	209	CG		A	98	37.635	10.342	-4.508	1.00 19.	
	ATOM	210		LEU		98	37.990	9.762	-3.146	1.00 20.	
	MOTA	211		LEU		98	36.143	10.627	-4.588	1.00 17.	
	MOTA	212	С	LEU		98	40.512	10.597	-5.677	1.00 17.	
	MOTA	213	0	LEU		98	40.527	10.920	-6.863	1.00 18.	
20	MOTA	214	N	ALA		99	40.995	9.438	-5.246	1.00 17.	
	MOTA	215	CA	ALA	Α	99	41.570	8.466	-6.168	1.00 18.	42 A
	MOTA	216	CB	ALA	Α	99	43.090	8.524	-6.105	1.00 14.	76 A
	MOTA	217	C	ALA	Α	99	41.102	7.055	-5.848	1.00 21.	40 A
	MOTA	218	0	ALA	Α	99	40.941	6.691	-4.679	1.00 22.	52 A
25	ATOM	219	N	ARG	Α	100	40.878	6.261	-6.888	1.00 19.	77 A
	ATOM	220	CA	ARG	Α	100	40.459	4.884	-6.693	1.00 20.	85 A
	ATOM	221	CB	ARG	А	100	39.202	4.585	-7.518	1.00 24.	22 A
	ATOM	222	CG	ARG	Α	100	38.608	3.205	-7.256	1.00 31.	78 A
	ATOM	223	CD	ARG			37.326	2.979	-8.048	1.00 36.	
30	ATOM	224	NE	ARG			36.213	3.818	-7.594	1.00 41.	
	ATOM	225	CZ	ARG			35.566	3.662	-6.439	1.00 42.	
	ATOM	226		ARG			35.912	2,696	-5.598	1.00 40.	
	ATOM	227		ARG			34.559	4.468	-6.128	1.00 43.	
	ATOM	228	C	ARG			41.613	3.985	-7.129	1.00 18.	
35	ATOM	229	ō	ARG			42.078	4.065	-8.271	1.00 19.	
55	ATOM	230	N			101	42.102	3.157	-6.212	1.00 16.	
	ATOM	231	CA			101	43.196	2.246	-6.533	1.00 16.	
	ATOM	232	CB			101	43.774	1.637	-5.248	1.00 16.	
	ATOM	233	CG			101	44.917	0.657	-5.488	1.00 16.	
40	ATOM	234	CD			101	45.501	0.115	-4.200	1.00 18.	
40	ATOM	235		GLU			44.733	-0.081	-3.239	1.00 18.	
	ATOM	236		GLU			46.725	-0.132	-4.150	1.00 17.	
	ATOM	237	C			101	42.625	1.152	-7.442	1.00 17.	
45	ATOM	238	0			101	41.681	0.462	-7.069	1.00 18.	
43	ATOM	239	N			102	43.198	1.002	-8.632	1.00 19.	
	ATOM	240	CA	LEU			42.718	0.025	-9.607	1.00 20.	
	MOTA	241	CB	LEU			43.569		-10.878	1.00 23.	
	MOTA	242	CG			102	43.531		-11.642	1.00 25.	
	MOTA	243		LEU			44.577		-12.748	1.00 27.	
50	MOTA	244		LEU			42.140		-12.214	1.00 26.	
	MOTA	245	C			102	42.671	-1.418	-9.125	1.00 21.	
	MOTA	246	0			102	41.668	-2.103	-9.305	1.00 21.	
	MOTA	247	N	ALA			43.753	-1.874	-8.507	1.00 19.	
	MOTA	248	CA	ALA			43.836	-3.249	-8.035	1.00 20.	
55	MOTA	249	CB	ALA			45.284	-3.571	-7.671	1.00 19.	
	MOTA	250	C	ALA			42.919	-3.629	-6.872	1.00 19.	
	MOTA	251	0			103	42.703	-4.815	-6.628	1.00 20.	
	MOTA	252	N			104	42.361	-2.643	-6.175	1.00 18.	
	ATOM	253	CA	THR	Α	104	41.517	-2.927	-5.018	1.00 17.	15 A

	ATOM	254	CB	THR	Α	104	42.212	-2.484	-3.717	1.00 19.54	A
	ATOM	255		THR			42.456	-1.070	-3.773	1.00 19.26	
	ATOM	256		THR			43.536	-3.219	-3.529	1.00 17.02	
	ATOM	257	C	THR			40.159	-2.247	-5.026	1.00 19.44	A
5	ATOM	258	ō	THR			39.259	-2.648	-4.285	1.00 18.70	
	ATOM	259	N	SER			40.034	-1.207	-5.847	1.00 19.65	
	ATOM	260	CA	SER			38.819	-0.400	-5.967	1.00 19.03	
	ATOM	261	CB	SER			37.598	-1.304	-6.173	1.00 21.81	
	ATOM	262	OG	SER			36.431	-0.539	-6.412	1.00 23.01	
10								0.447	-4.701	1.00 23.01	
10	MOTA	263	C	SER			38.644				
	MOTA	264	0	SER			37.602	1.070	-4.488	1.00 18.66	
	MOTA	265	N	ARG			39.674	0.468	-3.861	1.00 16.84	
	MOTA	266	CA	ARG			39.655	1.267	-2.634	1.00 16.21	
	ATOM	267	CB	ARG			40.827	0.886	-1.723	1.00 16.41	
15	MOTA	268	CG	ARG			40.619	-0.367	-0.906	1.00 15.49	
	MOTA	269	CD	ARG			41.887	-0.755	-0.170	1.00 17.43	
	MOTA	270	NE	ARG			41.620	-1.792	0.824	1.00 20.47	
	MOTA	271	CZ	ARG			42.548	-2.568	1.371	1.00 20.24	A
	MOTA	272		ARG			43.821	-2.433	1.017	1.00 17.80	
20	MOTA	273		ARG			42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	C	ARG	Α	106	39.785	2.746	-2.981	1.00 17.37	A
	MOTA	275	0	ARG	Α	106	40.514	3.103	-3.902	1.00 17.75	A
	MOTA	276	N	GLU	Α	107	39.085	3.599	-2.240	1.00 16.06	A
	ATOM	277	CA	GLU	Α	107	39.156	5.039	-2.461	1.00 20.80	A
25	ATOM	278	CB	GLU	Α	107	37.779	5.694	-2.337	1.00 22.93	A
	ATOM	279	CG	GLU	Α	107	36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD	GLU	Α	107	35.431	5.975	-3.148	1.00 32.40	A
	ATOM	281	OE1	GLU	Α	107	35.262	6.939	-3.923	1.00 33.74	A
	ATOM	282	OE2	GLU	Α	107	34.608	5.654	-2.263	1.00 36.00	A
30	ATOM	283	С	GLU	Α	107	40.053	5.678	-1.410	1.00 18.93	A
	ATOM	284	ò	GLU			39.891	5.427	-0.220	1.00 19.21	
	ATOM	285	N	TYR			40.988	6.507	-1.852	1.00 16.70	
	ATOM	286	CA	TYR			41.883	7.209	-0.942	1.00 15.86	
	ATOM	287	CB	TYR			43.325	6.728	-1.104	1.00 15.30	
35	ATOM	288	CG	TYR			43.593	5.328	-0.612	1.00 16.33	
	ATOM	289		TYR			43.765	5.066	0.746	1.00 16.36	
	ATOM	290		TYR			44.046	3.769	1.201	1.00 18.48	
	ATOM	291	CD2	TYR			43.701	4.268	-1.511	1.00 13.25	
	ATOM	292		TYR			43.980	2.981	-1.075	1.00 17.28	
40	ATOM	293	CZ	TYR			44.152	2.736	0.276	1.00 19.17	A
40	ATOM	294	OH	TYR			44.440	1.461	0.688	1.00 19.38	
	ATOM	295	C	TYR			41.850	8.687	-1.292	1.00 16.80	
	ATOM	296	o	TYR			41.560	9.058	-2.431	1.00 15.22	A
								9.528	-0.306	1.00 14.61	
45	ATOM	297	N	ALA			42.132				
43	ATOM	298	CA	ALA			42.207	10.957	-0.539	1.00 14.30	
	MOTA	299	CB	ALA			41.671	11.726	0.661	1.00 14.78	
	ATOM	300	C	ALA			43.713	11.136	-0.667	1.00 16.79	
	MOTA	301	0	ALA			44.450	10.983	0.317	1.00 16.52	
	MOTA	302	N	ILE			44.182	11.410	-1.881	1.00 14.80	
50	MOTA	303	CA	ILE			45.609	11.574	-2.093	1.00 15.80	
	MOTA	304	CB	ILE			46.065	10.863	-3.396	1.00 16.85	
	MOTA	305		ILE			47.550	11.098	-3.632	1.00 16.80	
	MOTA	306		ILE			45.774	9.358	-3.284	1.00 17.76	
	MOTA	307		ILE			46.308	8.513	-4.437	1.00 16.07	
55	MOTA	308	С	ILE			46.004	13.045	-2.129	1.00 17.78	
	MOTA	309	0	ILE			45.534	13.813	-2.976	1.00 16.24	
	MOTA	310	N	LYS			46.846	13.435	-1.177	1.00 16.15	
	ATOM	311	CA	LYS			47.326	14.808	-1.100	1.00 17.20	
	ATOM	312	CB	LYS	Α	111	47.700	15.176	0.344	1.00 17.41	A

	ATOM	313	CG	LYS	Α	111	48.350	16.547	0.464	1.00 20.	71 A
	ATOM	314	CD			111	48.585	16.971	1.910	1.00 24.3	
	ATOM	315	CE	LYS			47.288	17.381	2.598	1.00 29.	
	ATOM	316	NZ			111	47.516	17.866	4.000	1.00 30.	
5	ATOM	317	C	LYS			48.551	14.890	-1.994	1.00 16.	
	ATOM	318	ŏ			111	49.509	14.137	-1.813	1.00 18.2	
	ATOM	319	N			112	48.509	15.798	-2.963	1.00 15.1	
	ATOM	320	CA			112	49.606	15.967	-3.907	1.00 17.2	
1.0	ATOM	321	CB			112	49.079	15.911	-5.358	1.00 16.	
10	ATOM	322		ILE			50.235	15.998	-6.341	1.00 15.	
	MOTA	323		ILE			48.293	14.609	-5.565	1.00 16.	
	MOTA	324		ILE			47.580	14.511	-6.904	1.00 18.	
	MOTA	325	С			112	50.307	17.301	-3.663	1.00 19.0	
	MOTA	326	0			112	49.669	18.350	-3.635	1.00 19.	
15	MOTA	327	N			113	51.622	17.245	-3.472	1.00 20.3	
	MOTA	328	CA			113	52.416	18.442	-3.214	1.00 22.	
	ATOM	329	CB			113	52.995	18.397	-1.794	1.00 22.	13 A
	MOTA	330	CG	LEU	Α	113	52.042	18.063	-0.646	1.00 22.	46 A
	MOTA	331	CD1	LEU	Α	113	51.866	16.557	-0.553	1.00 23.0	31 A
20	MOTA	332	CD2	LEU	Α	113	52.603	18.595	0.660	1.00 23.0	68 A
	ATOM	333	C	LEU	Α	113	53.560	18.547	-4.215	1.00 23.3	37 A
	ATOM	334	0	LEU	Α	113	54.300	17.586	-4.424	1.00 23.3	11 A
	ATOM	335	N	GLU	Α	114	53.706	19.714	-4.834	1.00 23.4	38 A
	ATOM	336	CA			114	54.771	19.920	-5.806	1.00 26.0	
25	ATOM	337	CB			114	54.435	21.111	-6.706	1.00 27.	
	ATOM	338	CG			114	55.533	21.452	-7.696	1.00 35.0	
	ATOM	339	CD			114	55.220	22.696	-8.497	1.00 39.2	
	ATOM	340		GLU			54.808	23.703	-7.885	1.00 41.	
	ATOM	341		GLU			55.395	22.670	-9.736	1.00 44.0	
30	ATOM	342	C			114	56.087	20.163	-5.067	1.00 24.	
50	ATOM	343	ŏ			114	56.186	21.071	-4.238	1.00 24.	
	ATOM	344				115	57.096	19.350		1.00 24.	
		344	N CA			115			-5.360	1.00 24.	
	ATOM						58.376	19.493	-4.678		
2.5	ATOM	346	CB	LYS			59.339	18.373	-5.103	1.00 23.	
35	ATOM	347	CG			115	59.139	17.080	-4.308	1.00 23.0	
	ATOM	348	CD			115	60.064	15.944	-4.743	1.00 21.	
	MOTA	349	CE			115	59.691	15.400	-6.117	1.00 22.	
	MOTA	350	NZ			115	60.447	14.150	-6.448	1.00 19.	
	MOTA	351	С	LYS			59.031	20.858	-4.868	1.00 26.	
40	MOTA	352	0			115	59.492	21.469	-3.903	1.00 26.	
	MOTA	353	N	ARG			59.058	21.348	-6.102	1.00 28.	
	ATOM	354	CA	ARG			59.678	22.638	-6.380	1.00 29.	
	ATOM	355	CB	ARG	Α	116	59.533	22.980	-7.868	1.00 31.2	29 A
	MOTA	356	CG	ARG	Α	116	60.047	24.361	-8.267	1.00 33.	19 A
45	ATOM	357	CD	ARG	Α	116	61.368	24.710	-7.590	1.00 35.3	13 A
	MOTA	358	NE	ARG	Α	116	62.329	23.612	-7.618	1.00 36.	42 A
	MOTA	359	CZ	ARG	Α	116	63.510	23.648	-7.009	1.00 36.3	18 A
	ATOM	360	NH1	ARG	Α	116	63.871	24.729	-6.332	1.00 36.3	12 A
	MOTA	361	NH2	ARG	Α	116	64.324	22.602	-7.067	1.00 35.7	77 A
50	ATOM	362	С	ARG	Α	116	59.097	23.761	-5.519	1.00 29.	70 A
	ATOM	363	0	ARG	А	116	59.843	24.515	-4.889	1.00 29.3	16 A
	ATOM	364	N	HIS			57.773	23.862	-5.472	1.00 27.2	
	ATOM	365	CA	HIS			57.126	24.903	-4.681	1.00 26.	
	ATOM	366	CB	HIS			55.606	24.835	-4.848	1.00 28.	
55	ATOM	367	CG	HIS			54.881	26.005	-4.258	1.00 31.4	
22	ATOM	368		HIS			55.309	27.249	-3.935	1.00 33.	
	ATOM	369		HIS			53.536	25.974	-3.961	1.00 34.	
	ATOM	370		HIS			53.165	27.148	-3.480	1.00 34.	
	ATOM	371		HIS			54.222	27.140	-3.455	1.00 34.	
	MIUN	3/1	rer.Z	urs	м	11/	J4. LLL	41.040	0.400	1.00 33.	LU A

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	ATOM	372	C	HIS			57.477	24.780	-3.202		26.22	A
	ATOM	373	0	HIS	Α	117	57.737	25.776	-2.534	1.00	25.67	A
	ATOM	374	N	ILE	Α	118	57.469	23.554	-2.689	1.00	24.94	A
	ATOM	375	CA	ILE	Α	118	57.792	23.315	-1.285	1.00	23.94	A
5	ATOM	376	CB	ILE			57.711	21.812	-0.952		23.50	A
	ATOM	377		ILE			58.374	21.533	0.389		23.76	A
	ATOM	378		ILE			56.246	21.362	-0.959		24.42	A
	ATOM	379		ILE			56.066	19.858	-0.834		28.06	A
	MOTA	380	C	ILE			59.195	23.821	-0.958		23.78	A
10	ATOM	381	0	ILE	Α	118	59.402	24.495	0.048	1.00	23.49	A
	MOTA	382	N	ILE	Α	119	60.153	23.489	-1.815	1.00	23.46	A
	ATOM	383	CA	ILE	Α	119	61.534	23.913	-1.619	1.00	25.13	A
	ATOM	384	CB	ILE	Α	119	62.467	23.250	-2.664	1.00	24.25	A
	ATOM	385	CG2	ILE	А	119	63.858	23.890	-2.617	1.00	22.47	A
15	ATOM	386		ILE			62.540	21.738	-2.395		25.05	A
	ATOM	387		ILE			63.327	20.945	-3.439		24.62	A
	ATOM	388	C	ILE			61.667	25.435	-1.705		25.96	A
	MOTA	389	0	ILE			62.330	26.051	-0.872		24.78	A
	MOTA	390	N	LYS			61.028	26.039	-2.704		27.67	A
20	ATOM	391	CA	LYS			61.100	27.489	-2.879		30.29	A
	ATOM	392	CB	LYS	Α	120	60.242	27.940	-4.060	1.00	32.34	A.
	ATOM	393	CG	LYS	Α	120	60.674	27.407	-5.409	1.00	39.30	A
	ATOM	394	CD	LYS	Α	120	59.765	27.950	-6.512	1.00	45.19	A
	ATOM	395	CE	LYS	Α	120	58.294	27.636	-6.218	1.00	46.48	A
25	ATOM	396	NZ	LYS	А	120	57.363	28.155	-7.252	1.00	46.49	A
	ATOM	397	C	LYS			60.647	28.247	-1.638		30.89	A
	ATOM	398	ō	LYS			61.303	29.198	-1.217		32.48	A
	ATOM	399	N	GLU			59.527	27.825	-1.055		29.82	A
20	MOTA	400	CA	GLU			58.986	28.488	0.128		30.33	A
30	MOTA	401	CB	GLU			57.455	28.416	0.117		33.04	A
	MOTA	402	CG	GLU			56.794	29.021	-1.120		36.45	A
	ATOM	403	CD	GLU			57.221	30.456	-1.373	1.00	39.88	A
	MOTA	404	OE1	GLU	Α	121	57.200	31.264	-0.420	1.00	40.53	A
	ATOM	405	OE2	GLU	Α	121	57.573	30.778	-2.529	1.00	43.24	A
35	ATOM	406	С	GLU	Α	121	59.511	27.930	1.451	1.00	30.37	A
	ATOM	407	0	GLU	А	121	58.946	28.204	2.513	1.00	31.24	A
	ATOM	408	N	ASN			60.588	27.151	1.390		29.03	A
	ATOM	409	CA	ASN			61.183	26.573	2.594		28.46	A
	ATOM	410	CB	ASN			61.836	27.673	3.436		31.28	A
40	ATOM	411	CG	ASN			62.945	28.395	2.698		34.12	A A
40												
	ATOM	412		ASN			62.697	29.143	1.754		35.57	A
	MOTA	413		ASN			64.181	28.169	3.127		35.73	A
	ATOM	414	С	ASN			60.157	25.835	3.456		26.89	A
	ATOM	415	0	ASN			60.085	26.055	4.663		27.23	A
45	ATOM	416	N	LYS			59.375	24.955	2.842		23.99	A
	ATOM	417	CA	LYS	Α	123	58.358	24.210	3.574	1.00	22.43	A
	ATOM	418	CB	LYS	Α	123	57.031	24.248	2.810	1.00	21.97	A
	ATOM	419	CG	LYS	Α	123	56.475	25.645	2.599	1.00	25.68	A
	ATOM	420	CD	LYS	А	123	56.253	26.354	3.927	1.00	27.54	A
50	ATOM	421	CE	LYS			55.822	27.796	3.716		31.30	A
50	ATOM	422	NZ	LYS			55.756	28.540	5.004		33.21	A
	ATOM		C				58.748		3.821		22.20	A
		423		LYS				22.759				
	ATOM	424	0	LYS			57.924	21.960	4.264		22.50	A
	ATOM	425	N	VAL			59.997	22.412	3.535		20.59	A
55	MOTA	426	CA	VAL			60.439	21.039	3.730		20.25	A
	ATOM	427	CB	VAL	Α	124	61.922	20.850	3.328	1.00	19.43	A
	ATOM	428	CG1	VAL	Α	124	62.346	19.407	3.573	1.00	18.69	A
	ATOM	429		VAL			62.104	21.195	1.853		18.21	A
	ATOM	430	C	VAL			60.236	20.561	5.163		19.53	A
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	MOTA	431	0	VAL			59.841	19.418	5.385		20.02	A
	ATOM	432	N	PRO	А	125	60.513	21.422	6.159	1.00	20.01	A
	ATOM	433	CD	PRO	n	125	61.178	22.738	6.118	1 00	18.69	A
	MOTA	434	CA	PRO			60.318	20.979	7.544		19.88	A
5	ATOM	435	CB	PRO	Α	125	60.793	22.180	8.363	1.00	19.95	A
	MOTA	436	CG	PRO	A	125	61.839	22.805	7.479	1.00	18.85	A
	ATOM	437	c	PRO			58.848	20.642	7.824		19.76	A
	ATOM	438	0	PRO			58.544	19.700	8.550		16.99	A
	ATOM	439	N	TYR	Α	126	57.947	21.418	7.235	1.00	18.98	A
10	ATOM	440	CA	TYR	А	126	56.516	21.220	7.435	1.00	21.97	A
	ATOM	441	CB	TYR			55.752	22.448	6.933		25.17	A
	ATOM	442	CG	TYR	Α	126	56.040	23.690	7.748	1.00	30.98	A
	ATOM	443	CD1	TYR	Α	126	55.438	23.886	8.991	1.00	33.95	A
	ATOM	444	CE1	TYR	Δ	126	55.721	25.015	9.763	1 00	36.60	A
15	ATOM	445		TYR			56.938	24.657	7.292		35.43	A
13												
	MOTA	446	CE2	TYR	А	126	57.231	25.792	8.058	1.00	37.20	A
	MOTA	447	CZ	TYR	Α	126	56.618	25.962	9.291	1.00	37.40	A
	ATOM	448	OH	TYR	75	126	56.903	27.073	10.052	1 00	40.85	A
	MOTA	449	C	TYR			55.990	19.956	6.762		21.35	A
20	ATOM	450	0	TYR	Α	126	55.265	19.175	7.383	1.00	20.49	A
	ATOM	451	N	VAL	A	127	56.354	19.746	5.501	1.00	18.16	A
	ATOM	452	CA	VAL			55.892	18.562	4.790		17.58	A
	ATOM	453	CB	VAL			56.308	18.596	3.308		17.45	A
	ATOM	454	CG1	VAL	Α	127	55.786	17.350	2.600	1.00	17.97	A
25	ATOM	455	CG2	VAL	Δ	127	55.751	19.850	2.641	1 00	14.90	A
	ATOM	456	C	VAL			56.459	17.306	5.448		18.39	A
	ATOM	457	0	VAL	Α	127	55.769	16.298	5.583	1.00	18.14	A
	ATOM	458	N	THR	Α	128	57.716	17.381	5.869	1.00	17.50	A
	ATOM	459	CA	THR			58.375	16.260	6.530		18.54	A
30			CB	THR				16.586	6.805			
30	MOTA	460					59.861				18.01	A
	ATOM	461	OG1	THR	Α	128	60.537	16.804	5.559	1.00	21.14	A
	ATOM	462	CG2	THR	А	128	60.536	15.446	7.545	1.00	17.95	A
	ATOM	463	С	THR	70	128	57.676	15.941	7.856	1 00	19.49	A
	MOTA	464	0	THR			57.438	14.776	8.179		18.76	A
35	ATOM	465	N	ARG	Α	129	57.345	16.981	8.619	1.00	19.60	A
	ATOM	466	CA	ARG	А	129	56.673	16.804	9.904	1.00	20.12	A
	ATOM	467	CB	ARG			56.534	18.144	10.621		21.33	A
	ATOM							18.029	12.023			
		468	CG	ARG			55.948				28.02	A
	MOTA	469	CD	ARG	Α	129	55.721	19.404	12.597	1.00	31.25	A
40	ATOM	470	NE	ARG	А	129	56.940	20.205	12.560	1.00	37.78	A
	ATOM	471	CZ	ARG	Δ	129	56.962	21.524	12.391	1 00	40.10	A
	ATOM	472		ARG			55.828	22.197	12.239		40.03	
												A
	ATOM	473	NH2	ARG	Α	129	58.119	22.170	12.374	1.00	44.58	A
	ATOM	474	C	ARG	А	129	55.288	16.186	9.729	1.00	20.08	A
45	ATOM	475	0	ARG			54.891	15.305	10.496		20.40	A
75												
	MOTA	476	N	GLU			54.553	16.654	8.724		18.79	A
	MOTA	477	CA	GLU	Α	130	53.222	16.125	8.454	1.00	20.10	A
	ATOM	478	CB	GLU	A	130	52.638	16.749	7.183	1.00	19.92	A
	ATOM	479	CG	GLU			51.350	16.087	6.708		27.85	A
50												
30	MOTA	480	CD	GLU			50.581	16.933	5.707		29.72	A
	MOTA	481	OE1	GLU	Α	130	51.216	17.528	4.814	1.00	33.46	A
	ATOM	482	OE2	GLU	А	130	49.339	16.996	5.807	1.00	30.74	A
	ATOM	483	C	GLU			53.301	14.615	8.295		19.81	A
	ATOM	484	0	GLU			52.553	13.875	8.935		18.37	A
55	MOTA	485	N	ARG	Α	131	54.219	14.162	7.447	1.00	20.41	A
	MOTA	486	CA	ARG	Α	131	54.397	12.735	7.202	1.00	22.45	A
		487	CB	ARG					6.098			
	MOTA						55.442	12.511			25.16	A
	MOTA	488	CG	ARG			55.742	11.043	5.840		28.75	A
	ATOM	489	CD	ARG	Α	131	56.736	10.837	4.708	1.00	33.75	A

	ATOM	490	NE	ARG	А	131	57.020	9.415	4.520	1.00	10.07	A
	ATOM	491	CZ			131	57.756	8.915	3.532	1.00		A
	ATOM	492		ARG			58.293	9.721	2.625	1.00		A
	ATOM	493		ARG			57.955	7.606	3.449	1.00		A
5	ATOM	494	C			131	54.820	11.982	8.466	1.00 2		A
	ATOM	495	ŏ			131	54.241	10.948	8.804	1.00		A
	ATOM	496	N	ASP			55.831	12.497	9.160	1.00		A
	ATOM	497	CA	ASP			56.318	11.850	10.370	1.00		A
	ATOM	498	CB	ASP			57.570	12.564	10.888	1.00		A
10												
10	MOTA	499	CG	ASP			58.750	12.442	9.932	1.00		A
	MOTA	500		ASP			58.681	11.620	8.989	1.00		A
	MOTA	501		ASP			59.753	13.163	10.128	1.00 2		A
	MOTA	502	C			132	55.258	11.772	11.474	1.00		A
	ATOM	503	0			132	55.077	10.723	12.092	1.00		A
15	MOTA	504	N			133	54.551	12.868	11.725	1.00		A
	MOTA	505	CA			133	53.525	12.843	12.759	1.00		A
	ATOM	506	CB			133	52.908	14.244	12.990	1.00		A
	MOTA	507		VAL			51.708	14.135	13.918	1.00	L8.79	A
	MOTA	508	CG2	VAL	Α	133	53.953	15.180	13.604	1.00	L8.80	A
20	MOTA	509	C	VAL	Α	133	52.419	11.854	12.398	1.00	L9.46	A
	ATOM	510	0	VAL	Α	133	52.073	10.991	13.200	1.00	L9.94	A
	ATOM	511	N	MET	Α	134	51.878	11.957	11.187	1.00	19.15	A
	ATOM	512	CA	MET	Α	134	50.807	11.052	10.792	1.00 2	21.25	A
	ATOM	513	CB	MET	Α	134	50.309	11.381	9.383	1.00	17.34	A
25	ATOM	514	CG	MET			49.615	12.730	9.302	1.00		A
	MOTA	515	SD	MET			48.643	12.952	7.798	1.00		A
	ATOM	516	CE	MET			47.033	12.434	8.400	1.00		A
	ATOM	517	c	MET			51.203	9.582	10.881	1.00		A
	ATOM	518	o	MET			50.384	8.741	11.249	1.00		A
30	ATOM	519	N			135	52.454	9.273	10.556	1.00		A
50	ATOM	520	CA			135	52.939	7.895	10.615	1.00		A
	ATOM	521	CB			135	54.356	7.798		1.00		A
	ATOM	521	OG			135		8.177	10.039	1.00		A
							54.383		8.673			
2.5	ATOM	523	С			135	52.957	7.358	12.045	1.00		A
35	MOTA	524	0			135	52.926	6.148	12.261	1.00		A
	MOTA	525	N			136	53.014	8.261	13.018	1.00		A
	MOTA	526	CA			136	53.056	7.870	14.425	1.00		A
	MOTA	527	CB			136	53.823	8.914	15.238	1.00 2		A
	MOTA	528	CG	ARG			55.283	9.082	14.857	1.00		A
40	MOTA	529	CD			136	55.904	10.218	15.664	1.00		A
	MOTA	530	NE			136	55.602	10.073	17.084	1.00		A
	ATOM	531	CZ			136	55.867	10.990	18.007	1.00		A
	MOTA	532	NH1	ARG	Α	136	56.449	12.132	17.661	1.00	10.55	A
	MOTA	533	NH2	ARG	Α	136	55.540	10.769	19.276	1.00	36.72	A
45	ATOM	534	C	ARG	Α	136	51.667	7.709	15.036	1.00 2	26.38	A
	ATOM	535	0	ARG	Α	136	51.516	7.121	16.106	1.00 2	27.06	A
	ATOM	536	N	LEU	Α	137	50.655	8.235	14.360	1.00 2	24.77	A
	ATOM	537	CA	LEU	Α	137	49.294	8.162	14.870	1.00 2	24.70	A
	MOTA	538	CB	LEU	А	137	48.483	9.363	14.371	1.00		A
50	MOTA	539	CG			137	49.050	10.760	14.662	1.00 2		A
	ATOM	540		LEU			48.075	11.813	14.141	1.00		A
	ATOM	541		LEU			49.279	10.945	16.155	1.00		A
	ATOM	542	С			137	48.592	6.868	14.473	1.00 2		A
	ATOM	543	0			137	48.619	6.469	13.309	1.00 2		A
55	ATOM	544	N	ASP			47.971	6.218	15.451	1.00		A
55	ATOM	545	CA	ASP			47.239	4.977	15.219	1.00 2		A
	ATOM	546	CB	ASP				3.761		1.00 2		A
							48.124		15.523			
	MOTA	547	CG	ASP			47.432	2.448	15.201	1.00 2		A
	ATOM	548	ODI	ASP	Α	138	46.631	2.423	14.241	1.00 2	4./8	A

	ATOM				_				45 000			_
		549		ASP			47.691	1.443	15.897		25.39	A
	MOTA	550	C	ASP			46.031	4.991	16.138		20.47	A
	ATOM	551	0	ASP	Α	138	45.967	4.248	17.118	1.00	19.06	A
	ATOM	552	N	HIS	Α	139	45.075	5.852	15.810	1.00	18.27	A
5	ATOM	553	CA	HIS	А	139	43.869	6.016	16.606	1.00	18.21	A
	ATOM	554	CB	HIS			44.096	7.157	17.612		15.84	A
	ATOM	555	CG	HIS			42.985	7.332	18.600		15.24	A
	ATOM	556		HIS			42.884	6.964	19.900		13.97	A
	MOTA	557		HIS			41.791	7.943	18.280		14.74	A
10	MOTA	558		HIS			41.002	7.944	19.341		14.19	A
	ATOM	559	NE2	HIS			41.641	7.356	20.336		14.15	A
	ATOM	560	C	HIS	Α	139	42.715	6.330	15.654	1.00	18.50	A
	ATOM	561	0	HIS	Α	139	42.879	7.080	14.693	1.00	20.80	A
	ATOM	562	N	PRO	Α	140	41.527	5.767	15.913	1.00	18.32	A
15	ATOM	563	CD	PRO	А	140	41.143	4.984	17.100	1.00	16.71	A
	ATOM	564	CA	PRO			40.367	6.001	15.048		17.43	A
	ATOM	565	CB	PRO			39.273	5.157	15.704		16.64	A
							39.643	5.204	17.152		18.43	
	ATOM	566	CG	PRO								A
	MOTA	567	С	PRO			39.914	7.441	14.803		18.77	A
20	MOTA	568	0	PRO			39.207	7.695	13.831		19.88	A
	ATOM	569	N	PHE			40.301	8.381	15.664		17.14	A
	MOTA	570	CA	PHE	Α	141	39.874	9.767	15.477	1.00	16.42	A
	ATOM	571	CB	PHE	Α	141	39.568	10.422	16.836	1.00	14.60	A
	ATOM	572	CG	PHE	Α	141	38.386	9.817	17.556	1.00	15.26	A
25	ATOM	573	CD1	PHE	А	141	37.335	9.234	16.842	1.00	14.78	A
	ATOM	574		PHE			38.297	9.880	18.942		13.70	A
	ATOM	575		PHE			36.215	8.727	17.502		16.94	A
	ATOM	576		PHE			37.178	9.375	19.615		15.75	A
	MOTA	577	CZ	PHE			36.135	8.799	18.893		16.89	A
30	MOTA	578	Ç	PHE			40.857	10.641	14.694		16.15	A
	ATOM	579	0	PHE			40.799	11.871	14.761		17.35	A
	MOTA	580	N	PHE	Α	142	41.748	10.011	13.941	1.00	15.88	A
	ATOM	581	CA	PHE	Α	142	42.727	10.756	13.154	1.00	17.89	A
	ATOM	582	CB	PHE	Α	142	44.115	10.645	13.793	1.00	17.57	A
35	ATOM	583	CG	PHE	А	142	44.240	11.371	15.103	1.00	18.74	A
	ATOM	584		PHE			44.559	12.726	15.135		17.77	A
	ATOM	585		PHE			43.997	10.711	16.304		18.74	A
	ATOM	586		PHE			44.632	13.417	16.347		15.77	A
				PHE			44.065		17.522		17.56	
40	MOTA	587						11.393				A
40	MOTA	588	CZ	PHE			44.383	12.747	17.542		17.14	A
	MOTA	589	C	PHE			42.793	10.231	11.729		19.12	A
	ATOM	590	0	PHE			42.659	9.030	11.504		20.01	A
	MOTA	591	N	VAL	Α	143	42.978	11.135	10.769	1.00	18.72	A
	MOTA	592	CA	VAL	Α	143	43.102	10.735	9.371	1.00	18.52	A
45	ATOM	593	CB	VAL	Α	143	43.294	11.961	8.440	1.00	20.66	A
	ATOM	594	CG1	VAL	А	143	43.843	11.521	7.080	1.00	21.29	A
	ATOM	595		VAL			41.958	12.673	8.252		22.97	A
	ATOM	596	C	VAL			44.342	9.865	9.330		18.68	A
	ATOM	597	0	VAL			45.355	10.199	9.943		18.42	A
50												
50	MOTA	598	N	LYS			44.259	8.745	8.623		18.30	A
	MOTA	599	CA	LYS			45.384	7.824	8.535		18.78	A
	ATOM	600	CB	LYS	Α	144	44.889	6.373	8.608	1.00	22.27	A
	ATOM	601	CG	LYS	Α	144	46.017	5.340	8.557	1.00	29.72	A
	MOTA	602	CD	LYS	Α	144	45.491	3.912	8.674	1.00	34.16	A
55	ATOM	603	CE	LYS	А	144	46.631	2.896	8.577	1.00	37.67	A
	ATOM	604	NZ	LYS		144	46.138	1.484	8.629		39.02	A
	ATOM	605	C	LYS			46.192	8.002	7.261		18.53	A
	ATOM	606	0	LYS			45.643	8.314	6.200		18.18	A
	MOTA	607	N	LEU	А	142	47.502	7.816	7.385	1.00	16.79	A

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	ATOM	608	CA	LEU			48.411	7.900	6.251		17.45	A
	MOTA	609	CB	LEU			49.686	8.653	6.641		18.82	A
	MOTA	610	CG	LEU	Α	145	50.734	8.902	5.549	1.00	20.23	A
	ATOM	611	CD1	LEU	Α	145	51.836	9.799	6.093	1.00	18.83	A
5	ATOM	612	CD2	LEU	A	145	51.317	7.581	5.069	1.00	19.79	A
	ATOM	613	C	LEU			48.739	6.450	5.907		19.19	A
	ATOM	614	ŏ	LEU			49.451	5.772	6.659		17.36	A
		615		TYR			48.215	5.972	4.782		17.28	
	ATOM		N									A
	ATOM	616	CA	TYR			48.444	4.593	4.358		17.57	A
10	MOTA	617	CB	TYR			47.288	4.098	3.486		17.74	A
	ATOM	618	CG	TYR			45.981	3.926	4.214	1.00	17.50	A
	MOTA	619	CD1	TYR	Α	146	45.099	4.995	4.377	1.00	16.50	A
	ATOM	620	CE1	TYR	Α	146	43.881	4.827	5.039	1.00	17.10	A
	ATOM	621	CD2	TYR	Α	146	45.620	2.686	4.735	1.00	18.28	A
15	ATOM	622	CE2	TYR	A	146	44.411	2.506	5.399	1.00	19.84	A
	ATOM	623	CZ	TYR			43.547	3.576	5.544		17.53	A
	ATOM	624	OH	TYR			42.342	3.376	6.169		20.67	A
	ATOM	625	C	TYR			49.735	4.376	3.582		18.72	A
	MOTA	626	0	TYR			50.382	3.338	3.715		19.51	A
20	MOTA	627	N	PHE			50.110	5.350	2.765		18.09	A
	MOTA	628	CA	PHE	Α	147	51.307	5.203	1.952	1.00	17.20	A
	ATOM	629	CB	PHE	Α	147	51.007	4.258	0.783	1.00	16.77	A
	ATOM	630	CG	PHE	Α	147	49.835	4.699	-0.070	1.00	17.75	A
	ATOM	631		PHE			49.967	5.752	-0.975		16.58	A
25	ATOM	632		PHE			48.595	4.075	0.053		18.07	A
20	ATOM	633		PHE			48.886	6.178	-1.742		19.62	A
	ATOM	634		PHE			47.503	4.492	-0.710		18.56	A
	MOTA	635	CZ	PHE			47.647	5.546	-1.610		19.27	A
	ATOM	636	C	PHE			51.768	6.533	1.395		17.13	A
30	ATOM	637	0	PHE	Α	147	51.045	7.528	1.452		14.43	A
	MOTA	638	N	THR	Α	148	52.981	6.534	0.854	1.00	17.12	A.
	ATOM	639	CA	THR	Α	148	53.541	7.718	0.232	1.00	17.96	A
	MOTA	640	CB	THR	Α	148	54.449	8.531	1.197	1.00	21.51	A
	ATOM	641	og1	THR	А	148	55.605	7.760	1.537	1.00	18.83	A
35	ATOM	642		THR			53.700	8.897	2.472		19.60	A
33	ATOM	643	C	THR			54.386	7.262	-0.946		20.31	A
				THR								
	ATOM	644	0				54.860	6.124	-0.991		18.94	A
	ATOM	645	N	PHE			54.543	8.149	-1.916		19.16	A
	MOTA	646	CA	PHE			55.368	7.877	-3.073		18.01	A
40	MOTA	647	CB	PHE			54.748	6.801	-3.989		17.23	A
	MOTA	648	CG	PHE	Α	149	53.389	7.144	-4.544	1.00	16.88	A
	MOTA	649	CD1	PHE	Α	149	53.262	7.888	-5.712	1.00	18.58	A
	ATOM	650	CD2	PHE	Α	149	52.235	6.668	-3.927	1.00	17.31	A
	ATOM	651	CE1	PHE	Α	149	52.007	8.149	-6.267	1.00	19.26	A
45	ATOM	652	CE2	PHE	А	149	50.972	6.923	-4.470	1.00	19.17	A
	ATOM	653	CZ	PHE			50.858	7.663	-5.642		19.60	A
	ATOM	654	C	PHE			55.542	9.205	-3.774		20.85	A
	ATOM	655	0	PHE			54.934	10.200	-3.376		19.76	A
	ATOM	656	N	GLN			56.398	9.241	-4.782		19.79	A
50	MOTA	657	CA	GLN			56.636	10.481	-5.497		24.03	A
	MOTA	658	CB	GLN	Α	150	57.659	11.347	-4.739	1.00	24.45	A
	MOTA	659	CG	GLN	Α	150	58.986	10.645	-4.414	1.00	26.28	A
	ATOM	660	CD	GLN	Α	150	59.988	11.558	-3.692	1.00	29.02	A
	ATOM	661	OE1	GLN	А	150	60.693	12.353	-4.321	1.00	27.05	A
55	ATOM	662		GLN			60.042	11.449	-2.365		26.47	A
	ATOM	663	C	GLN		150	57.160	10.203	-6.885		23.88	A
	ATOM	664	0	GLN			57.673	9.118	-7.158		24.79	A
	ATOM	665	N	ASP			56.987	11.171	-7.774		25.88	A
	ATOM	666	CA	ASP	А	121	57.527	11.047	-9.117	1.00	26.49	A

	ATOM	667	CB	ASP	Α	151	56.437	11.126	-10.199	1.00	24.54	A
	ATOM	668	CG	ASP	Α	151	55.544	12.336	-10.064	1.00	24.95	A
	ATOM	669	OD1	ASP	Α	151	56.005	13.379	-9.561	1.00	22.44	A
	ATOM	670	OD2	ASP	Α	151	54.369	12.242	-10.490	1.00	25.72	A
5	ATOM	671	C	ASP	Α	151	58.515	12.203	-9.220	1.00	28.63	A
	MOTA	672	0	ASP	Α	151	58.890	12.780	-8.194	1.00	27.83	A
	ATOM	673	N	ASP			58.934		-10.426		29.21	A
	ATOM	674	CA	ASP	А	152	59.907		-10.562		31.88	A
	ATOM	675	CB	ASP			60.325		-12.026		33.94	A
10	ATOM	676	CG	ASP			61.033		-12.557		38.88	A
	ATOM	677		ASP			61.817		-11.791		39.67	A
	ATOM	678		ASP			60.817		-13.738		41.57	A
	ATOM	679	C	ASP			59.487		-10.013		30.90	A
	ATOM	680	o	ASP			60.316	15.735	-9.482		31.69	A
15	ATOM	681	N			153	58.207		-10.107		29.44	A
	ATOM	682	CA	GLU			57.767	16.632	-9.646		28.69	A
	ATOM	683	CB	GLU			56.984		-10.766		32.90	A
	ATOM	684	CG	GLU			57.451		-12.183		40.57	A
	ATOM	685	CD	GLU			56.920		-12.675		45.78	A
20	ATOM	686		GLU			55.682		-12.760		48.91	A
20	ATOM	687		GLU			57.736		-12.979		48.95	A
	ATOM	688	C	GLU			56.929	16.683	-8.372		26.43	A
	ATOM	689	0	GLU			56.947	17.688	-7.660		25.08	A
											22.39	A A
25	ATOM	690	N	LYS			56.205	15.610 15.631	-8.069 -6.912			
23	ATOM	691	CA				55.318		-7.398		21.43	A
	ATOM	692	CB	LYS			53.861	15.628			20.33	A
	ATOM	693	CG	LYS			53.505	16.716	-8.403		21.92	A A
	ATOM	694	CD	LYS			52.211		-9.146		19.70	
20	ATOM	695	CE	LYS			51.775		-10.077		20.04	A
30	ATOM	696	NZ	LYS			50.631	17.094	-10.951		19.97	A
	ATOM	697	С	LYS			55.458	14.522	-5.881		20.43	A
	ATOM	698	0	LYS			55.949	13.426	-6.173		21.13	A
	MOTA	699	N	LEU			54.985	14.832	-4.676		19.69	A
	MOTA	700	CA	LEU			54.950	13.900	-3.553		19.10	A
35	MOTA	701	CB	LEU			55.362	14.588	-2.252		19.65	A
	ATOM	702	CG	LEU			56.740	15.234	-2.129		21.20	A
	MOTA	703		LEU			56.848	15.918	-0.770		23.42	A
	MOTA	704		LEU			57.816	14.174	-2.277		23.08	A
40	MOTA	705	C			155	53.478	13.507	-3.427		18.87	A
40	MOTA	706	0	LEU			52.600	14.348	-3.620		18.61	A
	MOTA	707	N	TYR			53.209	12.249	-3.091		15.02	A
	MOTA	708	CA			156	51.834	11.783	-2.934		16.29	A
	MOTA	709	CB	TYR			51.470	10.769	-4.029		14.20	A
	MOTA	710	CG	TYR			51.603	11.273	-5.449		17.29	A
45	MOTA	711		TYR			52.857	11.429	-6.045		16.46	A
	MOTA	712		TYR			52.978	11.884	-7.360		18.68	A
	ATOM	713		TYR			50.474	11.588	-6.202		16.43	A
	ATOM	714		TYR			50.583	12.048	-7.512		16.31	A
	MOTA	715	CZ	TYR	Α	156	51.835	12.192	-8.083	1.00	18.17	A
50	MOTA	716	OH			156	51.941	12.651	-9.371		17.47	A
	MOTA	717	C	TYR	Α	156	51.657	11.108	-1.572	1.00	16.32	A
	ATOM	718	0	TYR	Α	156	52.412	10.197	-1.235		16.27	A
	MOTA	719	N	PHE			50.678	11.568	-0.792	1.00	15.47	A
	MOTA	720	CA	PHE			50.385	10.966	0.508		16.66	A
55	MOTA	721	CB	PHE	Α	157	50.324	12.014	1.629	1.00	16.91	A
	ATOM	722	CG	PHE	Α	157	51.631	12.708	1.907	1.00	18.96	A
	ATOM	723	CD1	PHE	Α	157	52.821	12.261	1.340	1.00	20.31	A
	ATOM	724	CD2	PHE	Α	157	51.664	13.829	2.732	1.00	21.12	A
	ATOM	725	CE1	PHE	Α	157	54.025	12.926	1.585	1.00	22.08	A

	ATOM	726	CE2	PHE	А	157	52.865	14.500	2.982	1.00 22.1	18 A
	ATOM	727	CZ			157	54.045	14.045	2.405	1.00 21.2	
	ATOM	728	C			157	49.016	10.308	0.404	1.00 16.5	
	ATOM	729	o			157	48.029	10.979	0.110	1.00 17.3	
5	ATOM	730	N			158	48.953	9.002	0.644	1.00 15.9	
,	ATOM	731	CA			158	47.684	8.299	0.572	1.00 16.	
	ATOM	732	C			158	47.000	8.383	1.920	1.00 14.9	
	MOTA	733	0	GLY			47.445	7.756	2.879	1.00 16.2	
	MOTA	734	N			159	45.915	9.145	1.989	1.00 13.	
10	MOTA	735	CA			159	45.191	9.340	3.241	1.00 15.2	
	MOTA	736	CB			159	45.031	10.835	3.517	1.00 14.2	
	ATOM	737	CG			159	46.270	11.726	3.385	1.00 19.0	
	MOTA	738		LEU			45.847	13.188	3.477	1.00 17.3	
	MOTA	739	CD2	LEU	Α	159	47.275	11.390	4.471	1.00 14.7	71 A
15	MOTA	740	C	LEU	Α	159	43.809	8.716	3.232	1.00 15.5	53 A
	ATOM	741	0	LEU	Α	159	43.232	8.472	2.177	1.00 16.0)5 A
	ATOM	742	N	SER	Α	160	43.268	8.469	4.418	1.00 15.8	36 A
	ATOM	743	CA	SER	Α	160	41.932	7.917	4.498	1.00 19.0)1 A
	ATOM	744	CB	SER	Α	160	41.566	7.582	5.949	1.00 22.9	90 A
20	ATOM	745	OG			160	41.901	8.629	6.833	1.00 24.	
	ATOM	746	C			160	40.987	8.968	3.924	1.00 20.4	
	ATOM	747	ō			160	41.213	10.173	4.062	1.00 19.9	
	ATOM	748	N			161	39.945	8.508	3.250	1.00 19.2	
	ATOM	749	CA			161	38.975	9.406	2.644	1.00 20.3	
25	ATOM	750	CB			161	38.471	8.785	1.332	1.00 20.0	
23		751	CG				37.314	9.502	0.666	1.00 20.7	
	ATOM	752		TYR		161					
	ATOM						37.222	10.895	0.682	1.00 18.2	
	MOTA	753		TYR			36.180	11.557	0.029	1.00 22.2	
	MOTA	754		TYR			36.333	8.784	-0.020	1.00 20.5	
30	MOTA	755	CE2	TYR			35.287	9.436	-0.678	1.00 24.2	
	MOTA	756	CZ			161	35.218	10.822	-0.648	1.00 22.3	
	MOTA	757	OH			161	34.194	11.471	-1.298	1.00 23.0	
	MOTA	758	C			161	37.812	9.681	3.598	1.00 20.3	
	ATOM	759	0			161	36.959	8.819	3.810	1.00 19.5	
35	MOTA	760	N	ALA	Α	162	37.791	10.880	4.178	1.00 19.9	92 A
	ATOM	761	CA	ALA	Α	162	36.721	11.271	5.099	1.00 21.0)7 A
	ATOM	762	CB	ALA	Α	162	37.187	12.419	6.002	1.00 19.6	50 A
	MOTA	763	С	ALA	A	162	35.542	11.712	4.238	1.00 22.0)7 A
	ATOM	764	0	ALA	Α	162	35.436	12.875	3.860	1.00 20.6	56 A
40	ATOM	765	N	LYS	Α	163	34.653	10.769	3.945	1.00 23.2	27 A
	ATOM	766	CA			163	33.503	11.017	3.080	1.00 27.1	
	ATOM	767	CB			163	32.663	9.741	2.963	1.00 29.6	
	ATOM	768	CG	LYS			33.455	8.524	2.515	1.00 37.6	
	ATOM	769	CD			163	32.556	7.310	2.321	1.00 42.2	
45	ATOM	770	CE			163	33.373	6.034	2.185	1.00 44.4	
75	ATOM	771	NZ			163	34.143	5.735	3.430	1.00 44.8	
	ATOM	772	C	LYS			32.581	12.186	3.411	1.00 25.7	
										1.00 26.5	
	ATOM	773	0	LYS			32.103	12.863	2.506		
50	MOTA	774	N	ASN			32.327	12.441	4.689	1.00 24.5	
50	MOTA	775	CA	ASN			31.420	13.522	5.033	1.00 23.7	
	MOTA	776	CB	ASN			30.610	13.129	6.265	1.00 25.0	
	MOTA	777	CG	ASN			29.537	12.101	5.932	1.00 27.5	
	ATOM	778		ASN			28.772	12.281	4.983	1.00 28.7	
	MOTA	779		ASN			29.475	11.024	6.704	1.00 27.1	
55	MOTA	780	C	ASN			31.999	14.931	5.169	1.00 24.4	
	ATOM	781	0	ASN			31.306	15.856	5.589	1.00 23.9	
	ATOM	782	N	GLY	Α	165	33.262	15.097	4.795	1.00 21.5	56 A
	ATOM	783	CA	GLY	Α	165	33.873	16.414	4.836	1.00 24.3	39 A
	ATOM	784	C	GLY	Α	165	34.191	17.043	6.181	1.00 23.6	52 A

	3.0001	705		OT 11	-	1.05	24 200	16 250	2 122	1 00	02.06	
	MOTA	785	0	GLY			34.380	16.352	7.177		23.26	A
	ATOM	786	N	GLU			34.234	18.373	6.186		23.22	A
	MOTA	787	CA	GLU	Α	166	34.563	19.176	7.362	1.00	24.54	A
	ATOM	788	CB	GLU	Α	166	35.055	20.558	6.913	1.00	25.04	A
5	ATOM	789	CG	GLU	A	166	36.419	20.569	6.229	1.00	26.48	A
	ATOM	790	CD	GLU			36.699	21.889	5.517		30.02	A
	ATOM	791		GLU			36.081	22.906	5.889		29.33	A
		792		GLU							30.48	
	MOTA						37.544	21.916	4.596			A
	MOTA	793	C	GLU			33.436	19.372	8.369		24.44	A
10	ATOM	794	0	GLU			32.279	19.541	8.001		22.76	A
	ATOM	795	N	LEU	Α	167	33.791	19.370	9.649	1.00	22.95	A
	MOTA	796	CA	LEU	Α	167	32.813	19.581	10.707	1.00	22.26	A
	ATOM	797	CB	LEU	Α	167	33.497	19.481	12.073	1.00	22.32	A
	ATOM	798	CG	LEU	Α	167	32.706	19.923	13.306	1.00	22.04	A
15	ATOM	799	CD1	LEU			31.454	19.074	13.463	1.00	19.66	A
	ATOM	800		LEU			33.597	19.805	14.537		21.17	A
	ATOM	801	C	LEU			32.193	20.971	10.529		23.49	A
							31.047	21.209	10.907		23.56	
	ATOM	802	0	LEU								A
	MOTA	803	N	LEU			32.960	21.887	9.948		24.25	A
20	MOTA	804	CA	LEU			32.473	23.245	9.722		26.64	A
	ATOM	805	CB	LEU			33.560	24.099	9.066		25.62	A
	MOTA	806	CG	LEU	Α	168	33.198	25.546	8.707	1.00	27.34	A
	ATOM	807	CD1	LEU	Α	168	32.718	26.296	9.946	1.00	26.42	A
	ATOM	808	CD2	LEU	Α	168	34.418	26.238	8.119	1.00	26.74	A
25	ATOM	809	C	LEU	А	168	31.234	23.218	8.829	1.00	27.13	A
	ATOM	810	ò	LEU			30.297	23.989	9.030		26.01	A
	ATOM	811	N	LYS			31.233	22.320	7.848		26.41	A
	ATOM	812	CA	LYS			30.106	22.210	6.934		27.70	A
20	ATOM	813	CB	LYS			30.324	21.064	5.945		30.49	A
30	MOTA	814	CG	LYS			29.151	20.854	4.993		32.47	A
	ATOM	815	CD	LYS			29.407	19.728	3.998		35.98	A
	MOTA	816	CE	LYS	Α	169	29.462	18.372	4.683	1.00	38.53	A
	MOTA	817	NZ	LYS	Α	169	29.622	17.263	3.702	1.00	41.00	A
	ATOM	818	C	LYS	Α	169	28.801	21.985	7.682	1.00	28.12	A
35	ATOM	819	0	LYS	А	169	27.785	22.608	7.371	1.00	28.08	A
	ATOM	820	N	TYR			28.826	21.094	8.668		26.53	A
	ATOM	821	CA	TYR			27.624	20.791	9.434		26.95	A
	ATOM	822	CB	TYR			27.810	19.476	10.193		25.03	A
	ATOM	823	CG	TYR			27.898	18.300	9.251		26.65	A
40	ATOM	824		TYR			26.745	17.661	8.790		28.27	
40												A
	MOTA	825		TYR			26.814	16.642	7.839		26.85	A
	MOTA	826		TYR			29.127	17.884	8.742		27.83	A
	ATOM	827		TYR			29.209	16.869	7.792		27.19	A
	MOTA	828	CZ	TYR			28.049	16.254	7.343		30.02	A
45	MOTA	829	OH	TYR	Α	170	28.130	15.268	6.382	1.00	29.23	A
	ATOM	830	C	TYR	Α	170	27.229	21.918	10.376	1.00	27.59	A
	ATOM	831	0	TYR	А	170	26.045	22.122	10.642	1.00	29.25	A
	ATOM	832	N	ILE			28.208	22.660	10.882		28.16	A
	ATOM	833	CA	ILE			27.883	23.770	11.763		29.03	A
50	ATOM	834	CB	ILE			29.151	24.435	12.337		27.51	A
50												
	MOTA	835		ILE			28.773	25.705	13.084		27.97	A
	MOTA	836		ILE			29.872	23.458	13.272		26.70	A
	MOTA	837		ILE			31.163	23.996	13.856		24.07	A
	MOTA	838	C	ILE			27.094	24.796	10.944		31.41	A
55	MOTA	839	0	ILE	Α	171	26.088	25.335	11.407	1.00	31.69	A
	ATOM	840	N	ARG	Α	172	27.546	25.047	9.719	1.00	33.21	A
	ATOM	841	CA	ARG			26.874	26.000	8.844	1.00	36.54	A
	ATOM	842	CB	ARG			27.734	26.314	7.616		37.73	A
	ATOM	843	CG	ARG			29.057	27.011	7.912		41.65	A
	111 011	343	56	21103	Λ	4.4			1.512	1.00	.1.03	А

	ATOM	844	CD	ARG	А	172	29.708	27.492	6.616	1.00 4	5.29	A
	ATOM	845	NE			172	31.037	28.070	6.812	1.00 4		A
	ATOM	846	CZ	ARG			31.314	29.059	7.658	1.00 5		A
	ATOM	847		ARG			30.355	29.593	8.406	1.00 5		A
5	ATOM	848		ARG			32.553	29.526	7.748	1.00 5		A
	ATOM	849	C	ARG			25.528	25.459	8.378	1.00 3		A
	ATOM	850	Ö	ARG			24.550	26.200	8.288	1.00 3		A
	ATOM	851	N	LYS			25.481	24.163	8.092	1.00 3		A
	ATOM	852	CA	LYS			24.259	23.528	7.619	1.00 3		A
10									7.272			
10	ATOM	853	CB			173	24.523	22.061		1.00 4		A
	MOTA	854	CG	LYS			23.279	21.298	6.830	1.00 4		A
	MOTA	855	CD	LYS			23.557	19.808	6.653	1.00 4		A
	MOTA	856	CE			173	24.477	19.530	5.469	1.00 5		A
	MOTA	857	NZ			173	23.855	19.894	4.160	1.00 5		A
15	MOTA	858	C			173	23.089	23.608	8.595	1.00 3		A
	MOTA	859	0	LYS			21.981	23.960	8.201	1.00 3		A
	MOTA	860	N	ILE	Α	174	23.320	23.282	9.863	1.00 3		A
	MOTA	861	CA	ILE	Α	174	22.229	23.314	10.833	1.00 3	7.36	A
	MOTA	862	CB			174	22.159	21.998	11.652	1.00 3	7.44	A.
20	MOTA	863	CG2	ILE	Α	174	22.058	20.802	10.709	1.00 3	8.37	A.
	MOTA	864	CG1	ILE	Α	174	23.397	21.850	12.532	1.00 3	7.25	A
	MOTA	865	CD1	ILE	Α	174	23.355	20.620	13.418	1.00 3	6.85	A
	ATOM	866	C	ILE	Α	174	22.259	24.492	11.801	1.00 3	6.71	A
	MOTA	867	0	ILE	Α	174	21.448	24.556	12.724	1.00 3	8.05	A
25	ATOM	868	N	GLY	Α	175	23.185	25.423	11.592	1.00 3	5.48	A
	ATOM	869	CA	GLY	А	175	23.265	26.585	12.462	1.00 3	5.29	A
	ATOM	870	С			175	24.053	26.360	13.737	1.00 3		A
	ATOM	871	0	GLY	А	175	25.066	27.019	13.970	1.00 3	7.46	A
	ATOM	872	N			176	23.581	25.441	14.571	1.00 3		A
30	ATOM	873	CA			176	24.253	25.113	15.822	1.00 3		A
	ATOM	874	CB			176	23.938	26.155	16.901	1.00 3		A
	ATOM	875	OG			176	22.599	26.056	17.347	1.00 3		A
	ATOM	876	c			176	23.796	23.731	16.276	1.00 3		A
	ATOM	877	ō			176	22.726	23.263	15.884	1.00 3		A
35	ATOM	878	N			177	24.609	23.085	17.103	1.00 2		A
33	ATOM	879	CA			177	24.313	21.743	17.597	1.00 2		A
	ATOM	880	CB			177	25.621	20.989	17.865	1.00 2		A
	ATOM	881	CG			177	26.372	20.585	16.622	1.00 2		A
40	ATOM	882		PHE			26.210	21.277	15.426	1.00 2		A
40	ATOM	883	CD2	PHE			27.266	19.516	16.662	1.00 2		A
	ATOM	884		PHE			26.923	20.912	14.290	1.00 2		A
	MOTA	885	CE2				27.986	19.143	15.532	1.00 2		A
	MOTA	886	CZ			177	27.815	19.841	14.343	1.00 2		A
	ATOM	887	C			177	23.500	21.752	18.884	1.00 2		A
45	MOTA	888	0			177	23.704	22.610	19.747	1.00 2		A
	MOTA	889	N	ASP			22.578	20.802	19.022	1.00 2		A
	MOTA	890	CA	ASP			21.816	20.729	20.260	1.00 2		A
	ATOM	891	CB	ASP			20.621	19.773	20.142	1.00 2		A
	ATOM	892	CG	ASP			21.020	18.372	19.720	1.00 3		A
50	MOTA	893		ASP			22.157	17.949	20.014	1.00 3		A
	MOTA	894		ASP			20.179	17.683	19.105	1.00 3		A
	MOTA	895	C	ASP	Α	178	22.810	20.228	21.311	1.00 2	5.03	A
	MOTA	896	0	ASP			23.974	19.968	20.992	1.00 2		A
	ATOM	897	N	GLU	Α	179	22.361	20.083	22.552	1.00 2	3.60	A
55	ATOM	898	CA	GLU	Α	179	23.247	19.644	23.619	1.00 2	5.18	A
	ATOM	899	CB	GLU	Α	179	22.542	19.770	24.971	1.00 2	7.60	A
	ATOM	900	CG	GLU	Α	179	23.324	19.176	26.130	1.00 3	2.58	A
	MOTA	901	CD	GLU	Α	179	22.997	19.845	27.449	1.00 3	5.82	A
	MOTA	902	OE1	GLU	Α	179	21.825	20.224	27.645	1.00 3	5.95	A

	ATOM	903	OE2	GLU			23.912	19.984	28.291	1.00 38.19	A
	MOTA	904	C	GLU	Α	179	23.808	18.235	23.450	1.00 24.08	A
	MOTA	905	0	GLU	Α	179	24.977	17.989	23.756	1.00 22.79	A
	ATOM	906	N	THR	Α	180	22.983	17.316	22.961	1.00 23.36	A
5	ATOM	907	CA	THR	Α	180	23.412	15.935	22.761	1.00 22.15	A
	MOTA	908	CB	THR	Α	180	22.224	15.054	22.320	1.00 23.77	A
	ATOM	909	OG1	THR	Α	180	21.222	15.075	23.341	1.00 26.37	A
	ATOM	910	CG2	THR	Α	180	22.670	13.616	22.088	1.00 22.66	A
	ATOM	911	C	THR	Α	180	24.533	15.830	21.724	1.00 22.01	A
10	ATOM	912	0	THR	Α	180	25.533	15.141	21.944	1.00 19.87	A
	ATOM	913	N	CYS	А	181	24.365	16.511	20.596	1.00 21.21	A
	ATOM	914	CA			181	25.372	16.480	19.541	1.00 22.22	A
	ATOM	915	CB	CYS	Α	181	24.800	17.065	18.250	1.00 24.62	A
	ATOM	916	SG	CYS	Α	181	23.435	16.080	17.560	1.00 29.50	A
15	ATOM	917	С	CYS	Α	181	26.633	17.232	19.954	1.00 23.07	A
	ATOM	918	0	CYS	Α	181	27.746	16.827	19.608	1.00 23.95	A
	ATOM	919	N	THR	А	182	26.463	18.325	20.695	1.00 22.76	A
	ATOM	920	CA			182	27.606	19.103	21.161	1.00 21.49	A
	ATOM	921	CB			182	27.167	20.346	21.978	1.00 21.37	A
20	ATOM	922	OG1	THR	Α	182	26.459	21.262	21.134	1.00 22.50	A
	ATOM	923	CG2	THR	Α	182	28.379	21.046	22.565	1.00 18.36	A
	ATOM	924	С	THR	А	182	28.454	18.215	22.071	1.00 21.48	A
	ATOM	925	0	THR	А	182	29.669	18.090	21.894	1.00 19.95	A
	ATOM	926	N	ARG			27.798	17.602	23.050	1.00 18.97	A
25	ATOM	927	CA	ARG			28.468	16.723	23.996	1.00 19.39	A
	ATOM	928	CB	ARG	А	183	27.455	16.140	24.984	1.00 19.46	A
	ATOM	929	CG	ARG	А	183	28.030	15.062	25.887	1.00 18.77	A
	ATOM	930	CD	ARG	Α	183	27.021	14.571	26.925	1.00 21.19	A
	ATOM	931	NE	ARG	Α	183	26.605	15.642	27.824	1.00 19.46	A
30	ATOM	932	CZ	ARG	Α	183	25.496	16.362	27.679	1.00 20.45	A
	ATOM	933	NH1	ARG	Α	183	24.672	16.123	26.666	1.00 19.81	A
	ATOM	934	NH2	ARG	Α	183	25.224	17.338	28.539	1.00 17.11	A
	ATOM	935	С	ARG	Α	183	29.206	15.577	23.302	1.00 20.02	A
	ATOM	936	0	ARG	Α	183	30.383	15.333	23.573	1.00 19.97	A
35	ATOM	937	N	PHE	Α	184	28.520	14.871	22.409	1.00 19.24	A
	ATOM	938	CA	PHE	Α	184	29.144	13.746	21.722	1.00 18.04	A
	ATOM	939	CB	PHE	Α	184	28.158	13.078	20.764	1.00 21.05	A
	MOTA	940	CG	PHE	A	184	28.719	11.857	20.098	1.00 22.67	A
	MOTA	941	CD1	PHE	Α	184	28.717	10.630	20.754	1.00 22.97	A
40	MOTA	942	CD2	PHE	Α	184	29.317	11.949	18.850	1.00 19.97	A
	ATOM	943	CE1	PHE	Α	184	29.308	9.510	20.176	1.00 23.53	A
	MOTA	944	CE2	PHE	Α	184	29.915	10.833	18.263	1.00 24.11	A
	ATOM	945	CZ	PHE	Α	184	29.910	9.613	18.928	1.00 22.97	A
	ATOM	946	C	PHE	A	184	30.403	14.127	20.941	1.00 17.99	A
45	ATOM	947	0	PHE	Α	184	31.461	13.531	21.130	1.00 18.89	A
	MOTA	948	N	TYR	Α	185	30.292	15.110	20.056	1.00 15.73	A
	ATOM	949	CA	TYR	Α	185	31.443	15.519	19.265	1.00 15.72	A
	MOTA	950	CB	TYR	Α	185	30.992	16.413	18.111	1.00 17.33	A
	ATOM	951	CG	TYR	A	185	30.364	15.584	17.015	1.00 19.37	A
50	MOTA	952	CD1	TYR	Α	185	31.159	14.809	16.168	1.00 16.53	A
	MOTA	953	CE1	TYR	Α	185	30.590	13.952	15.232	1.00 18.12	A
	ATOM	954	CD2	TYR	Α	185	28.976	15.484	16.892	1.00 18.18	A
	ATOM	955	CE2	TYR	Α	185	28.398	14.623	15.956	1.00 18.90	A
	MOTA	956	CZ			185	29.211	13.861	15.133	1.00 18.41	A
55	MOTA	957	OH			185	28.650	12.995	14.218	1.00 20.48	A
	ATOM	958	C			185	32.544	16.172	20.083	1.00 15.79	A
	ATOM	959	0	TYR	Α	185	33.720	16.015	19.766	1.00 17.69	A
	ATOM	960	N			186	32.176	16.887	21.142	1.00 15.68	A
	MOTA	961	CA	THR	Α	186	33.184	17.504	21.997	1.00 16.03	A

	ATOM	962	CB	THR	Α	186	32.559	18.403	23.094		16.62	A
	ATOM	963		THR			31.866	19.503	22.481		14.79	A
	MOTA	964		THR			33.656	18.953	24.019		14.68	A
	MOTA	965	C	THR	Α	186	33.954	16.375	22.680	1.00	15.59	A
5	ATOM	966	0	THR	Α	186	35.176	16.443	22.823	1.00	13.77	A
	MOTA	967	N	ALA	Α	187	33.234	15.333	23.097	1.00	14.06	A
	ATOM	968	CA	ALA	Α	187	33.869	14.196	23.757	1.00	14.74	A
	ATOM	969	CB	ALA	Α	187	32.810	13.195	24.224	1.00	14.32	A
	ATOM	970	C	ALA	Α	187	34.875	13.509	22.821	1.00	14.41	A
10	ATOM	971	0	ALA	Α	187	35.972	13.136	23.247	1.00	15.61	A
	MOTA	972	N	GLU	Α	188	34.516	13.340	21.549	1.00	14.01	A
	ATOM	973	CA	GLU	Α	188	35.443	12.704	20.615	1.00	13.50	A
	MOTA	974	CB	GLU	Α	188	34.782	12.449	19.251	1.00	12.85	A
	ATOM	975	CG	GLU	Α	188	33.622	11.454	19.282	1.00	12.71	A
15	ATOM	976	CD	GLU	Α	188	33.464	10.685	17.979	1.00	15.01	A
	ATOM	977	OE1	GLU	Α	188	33.687	11.275	16.899	1.00	13.21	A
	ATOM	978	OE2	GLU	Α	188	33.110	9.484	18.031	1.00	17.69	A
	ATOM	979	С			188	36.682	13.582	20.436		13.34	A
	ATOM	980	0	GLU	Α	188	37.803	13.085	20.408	1.00	14.69	A
20	ATOM	981	N	ILE	Α	189	36.486	14.893	20.326	1.00	13.52	A
	ATOM	982	CA	ILE	Α	189	37.627	15.787	20.159	1.00	13.35	A
	ATOM	983	CB	ILE	А	189	37.169	17.247	19.939	1.00	13.95	A
	ATOM	984		ILE			38.381	18.165	19.822		12.47	A
	ATOM	985		ILE		189	36.302	17.332	18.671		13.44	A
25	ATOM	986		ILE		189	35.588	18.664	18.491		14.29	A
	MOTA	987	C			189	38.530	15.702	21.394		14.63	A
	ATOM	988	0			189	39.753	15.595	21.271		12.97	A
	ATOM	989	N			190	37.927	15.751	22.582		14.35	A
	MOTA	990	CA	VAL	А	190	38.684	15.655	23.832	1.00	13.22	A
30	ATOM	991	CB	VAL		190	37.743	15.690	25.061		14.28	A
	MOTA	992		VAL			38.509	15.267	26.326		15.08	A
	ATOM	993		VAL			37.160	17.082	25.233		12.08	A
	ATOM	994	С	VAL	А	190	39.468	14.338	23.859	1.00	14.61	A
	ATOM	995	0			190	40.634	14.304	24.250		13.72	A
35	ATOM	996	N			191	38.825	13.254	23.432		15.26	A
	ATOM	997	CA	SER	Α	191	39.478	11.943	23.421	1.00	16.81	A
	ATOM	998	CB	SER	А	191	38.470	10.857	23.041	1.00	16.14	A
	ATOM	999	OG			191	39.018	9.569	23.238		16.94	A
	ATOM	1000	C	SER	Α	191	40.649	11.928	22.441	1.00	16.58	A
40	ATOM	1001	0	SER	Α	191	41.697	11.335	22.713	1.00	13.96	A
	ATOM	1002	N	ALA	Α	192	40.468	12.586	21.300	1.00	15.26	A
	ATOM	1003	CA	ALA			41.518	12.645	20.292		14.37	A
	ATOM	1004	CB	ALA	Α	192	40.989	13.296	19.016	1.00	14.43	A
	ATOM	1005	С	ALA	А	192	42.695	13.440	20.845	1.00	16.46	A
45	ATOM	1006	0	ALA	Α	192	43.851	13.038	20.697	1.00	17.96	A
	ATOM	1007	N	LEU			42.401	14.563	21.496		15.02	A
	ATOM	1008	CA	LEU			43.459	15.392	22.067		15.42	A
	ATOM	1009	CB	LEU	А	193	42.884	16.712	22.600	1.00	12.88	A
	ATOM	1010	CG			193	42.445	17.721	21.525		15.97	A
50	ATOM	1011		LEU			41.869	18.979	22.190		13.97	A
	ATOM	1012		LEU			43.642	18.088	20.655		14.58	A
	ATOM	1013	C			193	44.211	14.659	23.174		14.49	A
	ATOM	1014	ō			193	45.427	14.813	23.310		16.56	A
	ATOM	1015	N			194	43.500	13.870	23.975		13.96	A
55	ATOM	1016	CA			194	44.179	13.123	25.032		14.08	A
	ATOM	1017	CB			194	43.190	12.295	25.857		14.65	A
	ATOM	1018	CG			194	43.882	11.301	26.789		17.09	A
	ATOM	1019	CD			194	42.924	10.592	27.730		19.59	A
	ATOM	1020		GLU			41.809	10.237	27.295		19.25	A

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	ATOM	1021	OEZ	GLU	А	194	43.302	10.380	28.906		20.20	A
	ATOM	1022	C	GLU	Α	194	45.208	12.199	24.386	1.00	13.57	A
	ATOM	1023	0	GLU	'n	104	46.337	12.093	24.847	1 00	14.23	A
	MOTA	1024	N	TYR			44.822	11.544	23.301		14.89	A
5	ATOM	1025	CA	TYR	Α	195	45.743	10.642	22.618	1.00	16.58	A
	MOTA	1026	CB	TYR	A	195	45.030	9.910	21.488	1.00	17.29	A
	ATOM	1027	CG			195	45.956	9.058	20.649		17.92	A
	ATOM	1028	CD1	TYR	Α	195	46.347	7.788	21.077	1.00	17.96	A
	ATOM	1029	CE1	TYR	Α	195	47.203	6.996	20.304	1.00	19.77	A
10	MOTA	1030		TYR			46.445	9.524	19.428		16.67	A
10												
	MOTA	1031	CE2	TYR			47.299	8.744	18.650		18.51	A
	ATOM	1032	CZ	TYR	Α	195	47.671	7.481	19.094	1.00	20.24	A
	ATOM	1033	OH	TYR	А	195	48.506	6.705	18.325	1.00	21.89	A
	ATOM	1034	C			195	46.917	11.419	22.035		16.98	A
15	MOTA	1035	0	TYR			48.081	11.047	22.203		14.61	A
	ATOM	1036	N	LEU	Α	196	46.599	12.507	21.347	1.00	16.30	A
	ATOM	1037	CA	LEH	A	196	47.619	13.328	20.720	1.00	18.15	A
	ATOM	1038	CB	LEU			46.969	14.502	19.982		18.59	A
	ATOM	1039	CG	LEU	Α	196	47.834	15.203	18.935	1.00	22.51	A
20	ATOM	1040	CD1	LEU	Α	196	48.222	14.206	17.841	1.00	20.94	A
	ATOM	1041		LEU			47.060	16.375	18.338		22.98	A
	MOTA	1042	C			196	48.592	13.844	21.763		17.75	A
	ATOM	1043	0	LEU	Α	196	49.801	13.644	21.649	1.00	18.33	A
	ATOM	1044	N	HIS	А	197	48.064	14.495	22.792	1.00	17.12	A
25	ATOM	1045	CA	HIS			48.913	15.042	23.842		18.47	A
23												
	MOTA	1046	CB	HIS			48.069	15.866	24.817		15.90	A
	ATOM	1047	CG	HIS	Α	197	47.571	17.152	24.231	1.00	19.15	A
	ATOM	1048	CD2	HIS	A	197	47.830	17.745	23.038	1.00	18.22	A
				HIS			46.704	17.992			17.47	
	MOTA	1049							24.897			A
30	MOTA	1050	CEI	HIS	А	197	46.450	19.047	24.139	1.00	19.74	A
	ATOM	1051	NE2	HIS	Α	197	47.119	18.921	23.007	1.00	15.69	A
	ATOM	1052	С	HIS	Th.	197	49.696	13.958	24.572		19.40	A
	MOTA	1053	0	HIS			50.823	14.192	25.021		19.42	A
	ATOM	1054	N	GLY	Α	198	49.106	12.770	24.679	1.00	18.59	A
35	ATOM	1055	CA	GLY	Α	198	49.793	11.675	25.339	1.00	19.60	A
	ATOM	1056	C	GLY			51.075	11.307	24.612		21.86	A
	MOTA	1057	0	GLY			51.963	10.682	25.186		23.09	A
	MOTA	1058	N	LYS	Α	199	51.174	11.687	23.341	1.00	22.81	A
	ATOM	1059	CA	LYS	А	199	52.368	11.401	22.549	1.00	24.43	A
40	ATOM	1060	CB			199	51.990	10.905	21.154		26.00	A
70												
	MOTA	1061	CG	LYS			51.378	9.520	21.133		30.98	A
	MOTA	1062	CD	LYS	Α	199	51.291	9.002	19.708	1.00	36.85	A
	ATOM	1063	CE	LYS	А	199	50.832	7.559	19.682	1.00	40.37	A
	ATOM	1064	NZ	LYS			51.646	6.691	20.581		43.48	A
4.5												
45	MOTA	1065	C	LYS			53.253	12.631	22.414		23.88	A
	MOTA	1066	0	LYS	Α	199	54.144	12.669	21.568	1.00	24.97	A
	ATOM	1067	N	GLY	Δ	200	52.997	13.638	23.243	1.00	24.00	A
	ATOM	1068	CA	GLY			53.790	14.853	23.203		22.12	A
	MOTA	1069	C	GLY	А	200	53.665	15.632	21.907		22.14	A
50	MOTA	1070	0	GLY	Α	200	54.632	16.231	21.439	1.00	22.41	A
	ATOM	1071	N	TLE	a	201	52.475	15.630	21.320	1 00	20.00	A
	MOTA	1072	CA	ILE			52.252	16.355	20.080		18.93	A
	MOTA	1073	CB	ILE	Α	201	51.784	15.414	18.955	1.00	19.70	A
	ATOM	1074	CG2	ILE	Α	201	51.414	16.226	17.716	1.00	20.12	A
55	ATOM	1075		ILE			52.880	14.395	18.636		20.03	A
55												
	MOTA	1076		ILE			52.408	13.258	17.745		22.75	A
	ATOM	1077	C	ILE	Α	201	51.193	17.425	20.270	1.00	19.87	A
	ATOM	1078	0	ILE	Α	201	50.121	17.161	20.817	1.00	20.08	A
	ATOM	1079	N	ILE			51.508	18.633	19.815		19.94	A
	TITOTI	10/3	14	THE	Λ		21.300	10.000	20.013	1.00	20.07	А

	ATOM	1080	CA	ILE	Α	202	50.601	19.772	19.891	1.00	20.45	Α
	ATOM	1081	CB	ILE	Α	202	51.352	21.040	20.356	1.00	22.21	А
	ATOM	1082		ILE			50.381	22.220	20.470		22.67	A
	MOTA	1083		ILE			52.033	20.775	21.700		24.19	A
5	ATOM	1084		ILE			52.914	21.920	22.169		25.39	Α
	MOTA	1085	C	ILE	Α	202	50.105	19.999	18.464	1.00	20.71	A
	ATOM	1086	0	ILE	Α	202	50.910	20.067	17.538	1.00	19.48	A
	ATOM	1087	N	HIS			48.795	20.108	18.270		18.65	А
	ATOM	1088	CA	HIS			48.280	20.319	16.919		18.02	A
10												
10	MOTA	1089	CB	HIS			46.775	20.057	16.874		16.31	A
	MOTA	1090	CG	HIS			46.199	20.136	15.495		18.36	A
	ATOM	1091	CD2	HIS	Α	203	46.043	21.186	14.655	1.00	16.42	A
	ATOM	1092	ND1	HIS	Α	203	45.759	19.026	14.806	1.00	19.50	A
	ATOM	1093	CE1	HIS	А	203	45.359	19.389	13.600	1.00	17.64	A
15	ATOM	1094		HIS			45.522	20.694	13.483		20.87	A
15	ATOM	1095	C	HIS			48.589	21.738	16.405		18.92	A
	MOTA	1096	0	HIS			49.073	21.906	15.282		16.21	A
	MOTA	1097	N	ARG			48.301	22.744	17.232		18.60	A
	MOTA	1098	CA	ARG	Α	204	48.552	24.157	16.914	1.00	19.81	A
20	ATOM	1099	CB	ARG	Α	204	49.998	24.365	16.458	1.00	21.61	A
	ATOM	1100	CG	ARG	А	204	51.024	24.137	17.550	1.00	23.82	A
	ATOM	1101	CD	ARG			52.323	24.870	17.252		27.62	A
				ARG								
	MOTA	1102	NE				52.932	24.449	15.994		29.43	A
	MOTA	1103	CZ	ARG			54.125	24.861	15.572		33.10	A
25	ATOM	1104		ARG			54.835	25.706	16.311		32.12	A
	ATOM	1105	NH2	ARG	Α	204	54.614	24.426	14.418	1.00	30.25	A
	ATOM	1106	С	ARG	Α	204	47.624	24.830	15.905	1.00	20.03	A
	ATOM	1107	0	ARG	А	204	47.711	26.038	15.698	1.00	20.88	A
	ATOM	1108	N	ASP			46.755	24.071	15.255		18.96	A
30	ATOM	1109	CA	ASP			45.828	24.692	14.325		17.90	A
50			CB									
	ATOM	1110		ASP			46.418	24.741	12.914		18.95	A
	MOTA	1111	CG	ASP			45.655	25.688	12.008		20.36	A
	MOTA	1112		ASP			44.939	26.560	12.545		20.35	A
	MOTA	1113	OD2	ASP	Α	205	45.772	25.573	10.771	1.00	22.49	A
35	ATOM	1114	C	ASP	Α	205	44.500	23.956	14.328	1.00	19.60	A
	ATOM	1115	0	ASP	Α	205	43.876	23.751	13.287	1.00	21.53	A
	ATOM	1116	N	LEU			44.063	23.569	15.521		18.53	A
	ATOM	1117	CA	LEU			42.813	22.851	15.667		19.18	A
	ATOM	1118	CB	LEU			42.693	22.295	17.087		18.94	A
40	ATOM	1119	CG	LEU							23.10	A
40							41.511	21.358	17.346			
	MOTA	1120		LEU			41.615	20.142	16.436		23.01	A
	MOTA	1121		LEU			41.504	20.933	18.808		22.97	A
	MOTA	1122	C	LEU	Α	206	41.639	23.772	15.361	1.00	19.05	A
	ATOM	1123	0	LEU	Α	206	41.556	24.880	15.886	1.00	19.25	A
45	ATOM	1124	N	LYS	Α	207	40.740	23.307	14.500	1.00	17.54	A
	ATOM	1125	CA	LYS			39.564	24.081	14.110		18.60	A
	ATOM	1126	CB	LYS			39.980	25.248	13.196		18.98	A
	ATOM	1127	CG	LYS			40.786	24.817	11.982		18.20	A
	MOTA	1128	CD	LYS			41.246	26.000	11.139		21.42	A
50	MOTA	1129	CE	LYS	Α	207	42.223	25.537	10.062	1.00	23.21	A
	MOTA	1130	NZ	LYS	Α	207	42.561	26.604	9.084	1.00	29.61	A
	ATOM	1131	C	LYS	Α	207	38.566	23.181	13.388	1.00	18.18	A
	ATOM	1132	0	LYS	Α	207	38.921	22.100	12.915	1.00	18.11	A
	ATOM	1133	N	PRO			37.298	23.614	13.293		20.26	A
55	ATOM	1134	CD	PRO			36.713	24.833	13.882		18.79	A
55	ATOM	1135	CA	PRO			36.272	22.814	12.616		19.67	A
	MOTA	1136	СВ	PRO			35.063	23.742	12.608		19.45	A
	MOTA	1137	CG	PRO			35.231	24.509	13.891		21.81	A
	MOTA	1138	C	PRO	Α	208	36.674	22.372	11.209	1.00	21.04	A

	ATOM	1139	0	PRO	А	208	36.264	21.307	10.751	1.00	21.19	A
	ATOM	1140	N			209	37.474	23.188	10.528	1.00		A
	ATOM	1141	CA			209	37.928	22.872	9.170	1.00		A
	ATOM	1142	CB			209	38.644	24.084	8.558	1.00		A
5	ATOM	1143	CG			209	39.253	23.825	7.185	1.00		A
,	ATOM	1144	CD			209	40.155	24.958	6.716	1.00		A
	ATOM	1145		GLU			39,660	26.094	6.553	1.00		A
	MOTA	1146		GLU			41.363	24.711	6.511	1.00		A
	MOTA	1147	C			209	38.879	21.668	9.159	1.00		A
10	MOTA	1148	0			209	38.955	20.933	8.170	1.00		A
	MOTA	1149	N	ASN			39.600	21.490	10.263	1.00		A
	ATOM	1150	CA	ASN			40.574	20.412	10.436	1.00		A
	ATOM	1151	CB	ASN	Α	210	41.744	20.912	11.287	1.00	20.07	A
	ATOM	1152	CG	ASN	Α	210	42.746	21.698	10.479	1.00	25.77	A
15	MOTA	1153	OD1	ASN	Α	210	43.571	22.427	11.029	1.00	26.73	A
	ATOM	1154	ND2	ASN	Α	210	42.687	21.548	9.158	1.00	25.15	A
	MOTA	1155	C	ASN	Α	210	40.005	19.151	11.078	1.00	18.63	A
	ATOM	1156	0	ASN	Α	210	40.712	18.154	11.234	1.00	18.29	A
	ATOM	1157	N	ILE	Α	211	38.739	19.202	11.469	1.00	16.31	A
20	ATOM	1158	CA			211	38.090	18.058	12.085	1.00		A
	ATOM	1159	CB			211	37.336	18.488	13.354	1.00		A
	ATOM	1160		ILE			36.582	17.311	13.950	1.00		A
	ATOM	1161		ILE			38.342	19.046	14.365	1.00		A
	ATOM	1162		ILE			37.720	19.669	15.590	1.00		A
25	ATOM	1163	C			211	37.131	17.485	11.059	1.00		A
23	ATOM	1164	Ö			211	35.995	17.947	10.926	1.00		Ā
	ATOM	1165						16.486		1.00		
			N	LEU			37.599		10.317			A
	ATOM	1166	CA	LEU			36.784	15.875	9.274	1.00		A
	MOTA	1167	CB			212	37.685	15.249	8.202	1.00		A
30	ATOM	1168	CG			212	38.785	16.157	7.640	1.00		A
	MOTA	1169		LEU			39.476	15.450	6.485	1.00		A
	ATOM	1170		LEU			38.188	17.482	7.166	1.00		A
	MOTA	1171	C			212	35.843	14.825	9.837	1.00		A
	ATOM	1172	0	LEU			35.957	14.433	11.002	1.00		A
35	ATOM	1173	N	LEU	Α	213	34.915	14.368	9.000	1.00	17.84	A
	ATOM	1174	CA	LEU	Α	213	33.942	13.362	9.403	1.00	19.94	A
	ATOM	1175	CB	LEU	A	213	32.556	14.004	9.487	1.00	20.84	A
	ATOM	1176	CG	LEU	Α	213	32.396	15.059	10.583	1.00	20.31	A
	ATOM	1177	CD1	LEU	Α	213	31.124	15.837	10.367	1.00	22.75	A
40	MOTA	1178	CD2	LEU	Α	213	32.379	14.378	11.940	1.00	23.93	A
	ATOM	1179	С	LEU	А	213	33.914	12.187	8.426	1.00	20.98	A
	ATOM	1180	0	LEU	А	213	33.743	12.379	7.218	1.00	19.55	A
	ATOM	1181	N	ASN			34.088	10.970	8.935	1.00		A
	ATOM	1182	CA	ASN			34.055	9.814	8.049	1.00		A
45	ATOM	1183	CB	ASN			34.745	8.596	8.674	1.00		A
	ATOM	1184	CG	ASN			34.077	8.127	9.948	1.00		A
	ATOM	1185		ASN			32.908	8.422	10.206	1.00		A
	ATOM	1186		ASN			34.818	7.369	10.752	1.00		A
		1187	C						7.693	1.00		
50	MOTA			ASN			32.618	9.466				A
30	ATOM	1188	0	ASN			31.672	10.113	8.150	1.00		A
	ATOM	1189	N			215	32.459	8.433	6.879	1.00		A
	ATOM	1190	CA			215	31.138	8.003	6.445	1.00		A
	MOTA	1191	CB	GLU			31.275	6.796	5.513	1.00		A
	MOTA	1192	CG	GLU			29.970	6.334	4.896	1.00		A
55	MOTA	1193	CD			215	30.182	5.312	3.795	1.00		A
	MOTA	1194		GLU			30.817	4.268	4.065	1.00		A
	MOTA	1195	OE2				29.716	5.556	2.660	1.00		A
	MOTA	1196	C	GLU	Α	215	30.188	7.673	7.601	1.00	28.41	A
	ATOM	1197	0	GLU	Α	215	28.971	7.769	7.447	1.00	28.52	A

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	MOTA	1198	N	ASP	А	216	30.737	7.287	8.752	1.00	26.77	A
	ATOM	1199	CA	ASP	А	216	29.914	6.953	9.917	1.00	27.28	A
	MOTA	1200	CB	ASP	Α	216	30.538	5.795	10.696	1.00	31.27	A
	ATOM	1201	CG	ASP	Δ	216	30.390	4.466	9.979	1 00	37.61	A
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5	ATOM	1202	ODI	ASP	Α	216	29.274	4.170	9.499	1.00	39.45	A
	ATOM	1203	OD2	ASP	A	216	31.382	3.710	9.902	1.00	41.84	A
	MOTA	1204	C	ASP	А	216	29.697	8.135	10.862	1.00	26.37	A
	ATOM	1205	0	ASP	A	216	29.136	7.984	11.950	1.00	25.73	A
	ATOM	1206	N	MET			30.156	9.306	10.441		23.02	A
10	ATOM	1207	CA	MET	Α	217	30.015	10.527	11.218	1.00	21.83	A.
	ATOM	1208	CB	MET	75	217	28.537	10.789	11.517	1 00	23.24	A
	ATOM	1209	CG	MET	Α	217	27.742	11.186	10.274	1.00	22.98	A
	ATOM	1210	SD	MET	Δ	217	28.464	12.616	9.430	1 00	27.57	A
	MOTA	1211	CE	MET			27.679	13.974	10.332		26.68	A
15	ATOM	1212	C	MET	Α	217	30.844	10.618	12.502	1.00	21.51	A.
	ATOM	1213	ò	MET			30.474	11.323	13.440		18.62	A
	ATOM	1214	N	HIS	Α	218	31.957	9.892	12.544	1.00	20.10	A.
	ATOM	1215	CA	HIS	75	210	32.873	9.964	13.678	1 00	19.86	A
	MOTA	1216	CB	HIS	Α	218	33.482	8.594	13.977	1.00	20.21	A
20	ATOM	1217	CG	HIS	Δ	218	32.551	7.667	14.698	1 00	22.40	A
20												
	MOTA	1218	CD2	HIS	А	518	31.910	6.547	14.287	1.00	21.27	A
	ATOM	1219	ND1	HIS	А	218	32.177	7.863	16.011	1.00	19.59	A
	ATOM	1220		HIS			31.348	6.902	16.379		21.88	A
	ATOM	1221	NE2	HIS	Α	218	31.168	6.091	15.351	1.00	22.08	A
25	ATOM	1222	С	HIS	7.	219	33.947	10.921	13.172	1 00	19.10	A
23												
	ATOM	1223	0	HIS	Α	218	34.170	11.004	11.965	1.00	20.31	A
	MOTA	1224	N	ILE	A	219	34.617	11.638	14.067	1.00	17.21	A
	MOTA	1225	CA	ILE			35.628	12.586	13.618		15.26	A
	ATOM	1226	CB	ILE	Α	219	35.987	13.614	14.716	1.00	15.38	A.
30	ATOM	1227	CG2				34.722	14.305	15.221		14.58	
30												A
	MOTA	1228	CG1	ILE	Α	219	36.734	12.919	15.864	1.00	14.46	A
	ATOM	1229	CD1	ILE	75	210	37.279	13.885	16.911	1 00	13.74	A
	MOTA	1230	С	ILE	Α	219	36.929	11.944	13.161	1.00	16.21	A
	ATOM	1231	0	ILE	A	219	37.238	10.799	13.500	1.00	15.88	A
35	ATOM	1232					37.677	12.711			15.62	
33			N	GLN					12.378			A
	ATOM	1233	CA	GLN	Α	220	38.980	12.316	11.876	1.00	17.84	A
	MOTA	1234	CB	GLN	75	220	38.872	11.595	10.525	1 00	20.00	A
	MOTA	1235	CG	GLN	A	220	38.463	10.129	10.659	1.00	26.97	A
	MOTA	1236	CD	GLN	Δ	220	38.648	9.343	9.372	1 00	29.95	A
40												
40	MOTA	1237		GLN			37.968	9.590	8.373		33.12	A
	ATOM	1238	NE2	GLN	А	220	39.578	8.393	9.389	1.00	30.47	A.
	ATOM	1239	С	GLN			39.757	13.610	11.735		17.00	A
	ATOM	1240	0	GLN	Α	220	39.609	14.339	10.751	1.00	18.27	A.
	ATOM	1241	N	ILE	75	221	40.566	13.906	12.746	1 00	14.34	A
45	MOTA	1242	CA	ILE	Α	221	41.361	15.120	12.753	1.00	14.46	A
	ATOM	1243	CB	ILE	Δ	221	41.867	15.416	14.175	1 00	12.30	A
	MOTA	1244		ILE			42.764	16.656	14.167		14.78	A
	ATOM	1245	CG1	ILE	A	221	40.660	15.613	15.102	1.00	13.92	A
	ATOM	1246		ILE			41.003	15.901	16.543		15.06	A
50	MOTA	1247	C	ILE	Α	221	42.536	14.996	11.783	1.00	15.44	A
	ATOM	1248	0	ILE	70	221	43.106	13.915	11.613	1 00	13.93	A
	MOTA	1249	N	THR	Α	222	42.877	16.101	11.127	1.00	15.36	A
	ATOM	1250	CA	THR	Α	222	43.980	16.098	10.174	1.00	17.52	A
	MOTA	1251	CB	THR			43.470	15.836	8.750	1.00	19.92	A
55	ATOM	1252	OG1	THR	Α	222	44.587	15.637	7.875	1.00	18.78	A
			CG2									
	MOTA	1253					42.630	17.018	8.257		18.16	A
	ATOM	1254	C	THR	Α	222	44.735	17.428	10.192	1.00	19.60	A
	ATOM	1255	0	THR			44.509	18.257	11.084		18.59	A
	MOTA	1256	N	ASP	Α	223	45.630	17.610	9.216	1.00	18.69	A

	ATOM	1257	CA	ASP	Δ	223	46.440	18.825	9.069	1.00	20 12	A
	ATOM	1258	CB			223	45.532	20.065	9.108	1.00		A
		1259				223	46.248		8.670	1.00		A
	MOTA		CG					21.335				
	MOTA	1260		ASP			47.283	21.227	7.975	1.00		A
5	ATOM	1261		ASP			45.765	22.438	9.009	1.00		A
	MOTA	1262	C	ASP	Α	223	47.516	18.913	10.150	1.00	21.73	A
	ATOM	1263	0	ASP	Α	223	47.439	19.751	11.055	1.00	22.76	A
	ATOM	1264	N	PHE	Α	224	48.535	18.063	10.027	1.00	20.75	A
	ATOM	1265	CA			224	49.611	17.988	11.009	1.00		A
10	ATOM	1266	CB			224	49.805	16.527	11.424	1.00		A
	ATOM	1267	CG			224	48.682	15.991	12.263	1.00		A
	ATOM	1268		PHE			48.598	16.312	13.614	1.00		A
	MOTA	1269		PHE			47.681	15.212	11.693	1.00		A
	ATOM	1270		PHE			47.528	15.868	14.389	1.00		A
15	MOTA	1271		PHE			46.606	14.763	12.457	1.00		A
	MOTA	1272	CZ	PHE	Α	224	46.530	15.093	13.807	1.00	22.02	A
	MOTA	1273	C	PHE	Α	224	50.957	18.583	10.619	1.00	20.45	A
	ATOM	1274	0	PHE	Α	224	51.905	18.547	11.407	1.00	20.73	A
	ATOM	1275	N	GLY	Α	225	51.049	19.125	9.412	1.00	22.02	A
20	ATOM	1276	CA			225	52.301	19.713	8.981	1.00		A
	ATOM	1277	C			225	52.742	20.822	9.920	1.00		A
	ATOM	1278	o			225	53.939	21.041	10.122	1.00		A
	ATOM	1279	N			226	51.779	21.524	10.508	1.00		A
	MOTA	1280	CA			226	52.106	22.613	11.416	1.00		A
25	ATOM	1281	CB			226	51.199	23.829	11.160	1.00		A
	ATOM	1282	OG1	THR	Α	226	49.831	23.410	11.113	1.00	22.68	A
	MOTA	1283	CG2	THR	Α	226	51.571	24.490	9.834	1.00	25.00	A
	ATOM	1284	C	THR	Α	226	52.046	22.233	12.894	1.00	25.79	A
	ATOM	1285	0	THR	Α	226	52.019	23.100	13.768	1.00	24.54	A
30	ATOM	1286	N	ALA			52.037	20.935	13.173	1.00		A
	ATOM	1287	CA	ALA			52.004	20.475	14.550	1.00		A
	ATOM	1288	CB	ALA			51.659	18.993	14.607	1.00		A
	ATOM	1289	C	ALA			53.384	20.715	15.149	1.00		A
		1290	0									
2.5	ATOM			ALA			54.331	21.047	14.435	1.00		A
35	MOTA	1291	N			228	53.491	20.558	16.461	1.00		A
	MOTA	1292	CA	LYS			54.760	20.745	17.149	1.00		A
	MOTA	1293	CB	LYS			54.699	21.974	18.054	1.00		A
	MOTA	1294	CG	LYS	Α	228	56.007	22.294	18.765	1.00	41.23	A
	MOTA	1295	CD	LYS	Α	228	57.082	22.725	17.768	1.00	47.57	A
40	ATOM	1296	CE	LYS	Α	228	58.401	23.056	18.462	1.00	49.82	A
	ATOM	1297	NZ	LYS	А	228	59.459	23.425	17.480	1.00	51.49	A
	ATOM	1298	С			228	55.019	19.504	17.985	1.00		A
	ATOM	1299	ō			228	54.190	19.129	18.815	1.00		A
	ATOM	1300	N	VAL			56.159	18.860	17.756	1.00		A
45	ATOM	1301	CA			229	56.516	17.661	18.501	1.00		A
43												
	MOTA	1302	CB			229	57.248	16.646	17.609	1.00		A
	MOTA	1303		VAL			57.619	15.419	18.415	1.00		A
	MOTA	1304		VAL			56.370	16.264	16.436	1.00		A
	MOTA	1305	C			229	57.420	18.035	19.668	1.00		A
50	MOTA	1306	0	VAL	Α	229	58.581	18.392	19.474	1.00	35.91	A
	ATOM	1307	N	LEU	Α	230	56.877	17.948	20.878	1.00	40.57	A
	ATOM	1308	CA	LEU	А	230	57.615	18.289	22.088	1.00	46.10	A
	ATOM	1309	СВ			230	56.654	18.417	23.270	1.00		A
	ATOM	1310	CG			230	55.627	19.545	23.207	1.00		A
55	ATOM	1311		LEU			54.673	19.430	24.383	1.00		A
55												
	MOTA	1312		LEU			56.340	20.885	23.214	1.00		A
	ATOM	1313	С			230	58.695	17.279	22.440	1.00		A
	MOTA	1314	0			230	58.603	16.104	22.089	1.00		A
	MOTA	1315	N	SER	Α	231	59.717	17.756	23.145	1.00	55.81	A

	ATOM	1316	CA	SER	Α	231	60.824	16.914	23.583	1.00	61.14	Α
	ATOM	1317	CB	SER	Α	231	62.077	17.200	22.750	1.00	61.27	A
	ATOM	1318	OG	SER	Α	231	62.444	18.568	22.823	1.00	62.85	Α
	ATOM	1319	С	SER			61.124	17.126	25.071		64.65	A
5												
3	ATOM	1320	0			231	61.392	16.164	25.794		65.70	A
	MOTA	1321	N	PRO			61.081	18.387	25.549		67.54	A
	ATOM	1322	CD	PRO	Α	232	60.854	19.651	24.823	1.00	68.60	A
	ATOM	1323	CA	PRO	Α	232	61.358	18.655	26.966	1.00	68.74	A
	ATOM	1324	CB	PRO	Α	232	61.109	20.158	27.086	1.00	68.83	A
10	ATOM	1325	CG	PRO	А	232	61.505	20.666	25.737		68.96	A
	ATOM	1326	c	PRO			60.460	17.846	27.899		69.17	A
	ATOM	1327	Ö	PRO			59.335	17.494	27.541		69.94	A
	MOTA	1328	N	ALA			57.424	23.198	27.637		80.06	A
	ATOM	1329	CA	ALA			56.783	23.047	26.335		79.29	A
15	MOTA	1330	CB	ALA			55.275	22.907	26.512		78.64	A
	ATOM	1331	С	ALA	Α	237	57.092	24.239	25.433	1.00	79.07	A
	ATOM	1332	0	ALA	Α	237	56.250	25.113	25.249	1.00	79.47	A
	ATOM	1333	N	ALA	Α	238	58.297	24.280	24.871	1.00	78.57	A
	ATOM	1334	CA	ALA	А	238	58.683	25.383	23.992	1.00	78.50	A
20	ATOM	1335	CB	ALA			60.186	25.347	23.728		78.50	A
20	ATOM	1336	C	ALA			57.920	25.327	22.673		78.15	A
		1337		ALA							77.96	
	ATOM		0				57.243	24.341	22.375			A
	ATOM	1338	N	ALA			58.027	26.393	21.887		77.28	A
	MOTA	1339	CA	ALA			57.338	26.452	20.603		76.27	A
25	MOTA	1340	CB	ALA	Α	239	55.849	26.489	20.827		76.61	A
	MOTA	1341	C	ALA	Α	239	57.766	27.667	19.793	1.00	75.38	A.
	ATOM	1342	0	ALA	Α	239	58.955	27.955	19.700	1.00	75.89	A
	MOTA	1343	N	ASN	Α	240	56.781	28.357	19.214	1.00	73.95	A
	ATOM	1344	CA	ASN			56.967	29.553	18.389		71.07	A
30	ATOM	1345	CB	ASN			58.151	30.400	18.874		71.47	A
50	ATOM	1346	CG	ASN			59.459	30.055	18.174		72.06	A
	ATOM	1347		ASN			59.575	30.149	16.943		72.03	A
	MOTA	1348		ASN			60.470	29.665	18.964		71.91	A
	MOTA	1349	C	ASN			57.188	29.178	16.928		69.41	A
35	ATOM	1350	0	ASN	Α	240	57.480	28.024	16.624	1.00	70.09	A
	ATOM	1351	N	ALA	Α	241	57.055	30.165	16.038	1.00	66.62	A.
	ATOM	1352	CA	ALA	Α	241	57.246	30.013	14.585	1.00	63.94	A
	MOTA	1353	C	ALA	Α	241	55.952	30.080	13.772	1.00	60.63	A
	ATOM	1354	0	ALA	А	241	55.840	30.880	12.845	1.00	61.29	A
40	ATOM	1355	CB	ALA			57.979	28.704	14.246		65.23	A
	ATOM	1356	N	PHE			54.984	29.236	14.113		56.72	A
	ATOM	1357	CA	PHE			53.712	29.196	13.394		52.53	A
	ATOM	1358	CB	PHE			53.419	27.767	12.923		49.14	A
	MOTA	1359	CG	PHE			52.040	27.590	12.354		47.38	A
45	MOTA	1360		PHE			51.731	28.067	11.085		47.69	A
	MOTA	1361	CD2	PHE	Α	242	51.038	26.975	13.102	1.00	45.45	A.
	ATOM	1362	CE1	PHE	Α	242	50.445	27.937	10.565	1.00	46.75	A
	ATOM	1363	CE2	PHE	Α	242	49.751	26.840	12.594	1.00	45.41	A
	ATOM	1364	CZ	PHE	А	242	49.453	27.323	11.322	1.00	46.55	A
50	ATOM	1365	c	PHE			52.534	29.688	14.229		50.08	A
50	ATOM	1366	ō	PHE			52.502	29.505	15.444		49.86	A
	ATOM	1367	N	VAL			51.566	30.305	13.557		47.67	A
	ATOM	1368	CA	VAL			50.355	30.809	14.200		46.21	A
	MOTA	1369	CB			243	50.340	32.352	14.258		47.36	A
55	MOTA	1370		VAL			49.012	32.844	14.825		47.54	A
	MOTA	1371	CG2	VAL	Α	243	51.497	32.842	15.109	1.00	48.50	A
	ATOM	1372	C	VAL	Α	243	49.150	30.342	13.389	1.00	44.12	A
	ATOM	1373	0	VAL	Α	243	48.956	30.765	12.247	1.00	44.46	A
	ATOM	1374	N	GLY			48.348	29.467	13.985		40.48	Α
				-	-							-

	3.0007	1375		OT 11	-	244	47.176	28.941	13.306	1.00	27 65	-
	ATOM		CA									A
	ATOM	1376	C	GLY	Α	244	46.101	29.960	12.964	1.00		A
	ATOM	1377	0	GLY	Α	244	46.313	31.168	13.065	1.00	35.92	A
	ATOM	1378	N	THE	Δ	245	44.936	29.463	12.560	1.00	33 30	A
5												
	MOTA	1379	CA			245	43.813	30.312	12.184	1.00		A
	MOTA	1380	CB	THR	Α	245	42.593	29.450	11.829	1.00	32.00	A
	ATOM	1381	OG1	THR	Α	245	42.952	28.573	10.755	1.00	32.81	A
	ATOM	1382	CG2	THR	Δ	245	41.419	30.319	11.390	1.00	28 34	A
	ATOM	1383	C			245	43.476	31.296	13.296	1.00		A
10	MOTA	1384	0			245	43.212	30.907	14.434	1.00		A
	MOTA	1385	N	ALA	Α	246	43.486	32.576	12.938	1.00	25.22	A
	ATOM	1386	CA	ALA	Α	246	43.247	33.675	13.867	1.00	23.27	A.
	ATOM	1387	CB	ALA	А	246	42.956	34.955	13.082	1.00	22.94	A
	ATOM	1388	c	ALA			42.178	33.475	14.934	1.00		A
1.5												
15	MOTA	1389	0	ALA			42.431	33.705	16.114	1.00		A
	ATOM	1390	N			247	40.988	33.047	14.536	1.00		A
	MOTA	1391	CA	GLN	Α	247	39.911	32.886	15.504	1.00	20.17	A
	ATOM	1392	CB	GLN	Α	247	38.608	32.535	14.779	1.00	21.89	A
	ATOM	1393	CG			247	38.522	33.076	13.355	1.00		A
20	ATOM	1394	CD			247	37.220	33.794	13.064	1.00		A
20												
	MOTA	1395		GLN			36.172	33.447	13.605	1.00		A
	MOTA	1396	NE2	GLN	Α	247	37.278	34.792	12.189	1.00	28.70	A
	ATOM	1397	C	GLN	Α	247	40.181	31.849	16.595	1.00	19.43	A.
	ATOM	1398	0	GT.N	А	247	39.546	31.883	17.648	1.00	18.93	A
25	ATOM	1399	N			248	41.132	30.948	16.359	1.00		A
23												
	ATOM	1400	CA			248	41.441	29.896	17.329	1.00		A
	MOTA	1401	CB	TYR	Α	248	41.333	28.529	16.642	1.00	17.53	A
	MOTA	1402	CG	TYR	Α	248	40.013	28.362	15.927	1.00	19.32	A
	ATOM	1403	CD1	TYR	А	248	38.859	28.010	16.625	1.00	17.69	A
30	ATOM	1404	CE1	TYR			37.617	27.976	15.990	1.00		A
50												
	ATOM	1405	CD2	TYR			39.897	28.664	14.569	1.00		A
	ATOM	1406	CE2	TYR			38.665	28.635	13.924	1.00		A
	MOTA	1407	CZ	TYR	Α	248	37.527	28.295	14.643	1.00	19.46	A
	MOTA	1408	OH	TYR	Α	248	36.299	28.311	14.023	1.00	18.98	A
35	ATOM	1409	С	TYR	А	248	42.810	30.039	17.993	1.00	20.42	A
	ATOM	1410	ō			248	43.208	29.191	18.792	1.00		A
	MOTA	1411	N			249	43.523	31.114	17.673	1.00		A
	MOTA	1412	CA			249	44.841	31.343	18.251	1.00		A
	MOTA	1413	CB	VAL	Α	249	45.542	32.532	17.570	1.00	21.18	A
40	MOTA	1414	CG1	VAL	Α	249	46.821	32.896	18.317	1.00	22.45	A
	ATOM	1415		VAL			45.862	32.170	16.139	1.00		A
	ATOM	1416	C			249	44.764	31.606	19.750	1.00		A
	MOTA	1417	0			249	43.915	32.368	20.216	1.00		A
	MOTA	1418	N			250	45.654	30.965	20.503	1.00		A
45	ATOM	1419	CA	SER	Α	250	45.697	31.133	21.951	1.00	21.65	A
	ATOM	1420	CB	SER	A	250	46.370	29.919	22.613	1.00	22.02	A
	ATOM	1421	OG			250	47.692	29.725	22.132	1.00		A
	MOTA	1422	С			250	46.476	32.402	22.280	1.00		A
	MOTA	1423	0	SER	Α	250	47.332	32.828	21.511	1.00		A
50	MOTA	1424	N	PRO	Α	251	46.180	33.029	23.425	1.00	22.23	A
	ATOM	1425	CD	PRO	Α	251	45.163	32.684	24.433	1.00	22.97	A
	MOTA	1426	CA	PRO	A	251	46.893	34.254	23.800	1.00	22.52	A
		1427				251		34.650		1.00		
	ATOM		CB				46.233		25.127			A
	ATOM	1428	CG			251	45.726	33.329	25.676	1.00		A
55	ATOM	1429	С	PRO	Α	251	48.414	34.115	23.907	1.00	22.15	A
	ATOM	1430	0	PRO	Α	251	49.143	35.047	23.563	1.00	22.62	A
	ATOM	1431	N			252	48.901	32.966	24.367	1.00		A
	ATOM	1432	CA			252	50.347	32.772	24.500	1.00		A
	ATOM	1433	CB	GTIO	Α	252	50.673	31.382	25.071	1.00	20.59	A

	ATOM	1434	CG	GLU	А	252	49.993	30.232	24.352	1.00	21.91	A
	ATOM	1435	CD	GLU			48.691	29.822	25.014		21.51	A
	ATOM	1436		GLU			47.989	30.707	25.550		21.46	A
	ATOM	1437		GLU			48.367	28.613	24.993		20.23	A
5	ATOM	1438	C	GLU			51.071	32.970	23.167		22.99	A
,	ATOM	1439	Ö	GLU			52.191	33.480	23.136		23.17	A
	ATOM	1440	N	LEU			50.441	32.576	22.064		23.00	A
	ATOM	1441	CA	LEU			51.068	32.753	20.758		25.62	A
10	ATOM	1442	CB	LEU			50.277	32.029	19.669		26.75	A
10	MOTA	1443	CG	LEU			50.743	30.620	19.296		31.87	A
	MOTA	1444		LEU			50.433	29.651	20.422		31.81	A
	MOTA	1445		LEU			50.044	30.179	18.015		31.86	A
	MOTA	1446	C	LEU			51.201	34.228	20.371		26.94	A
	ATOM	1447	0	LEU .			52.107	34.601	19.626		27.09	A
15	ATOM	1448	N	LEU .			50.297	35.059	20.877		25.83	A
	MOTA	1449	CA	LEU .	Α	254	50.297	36.485	20.564	1.00	27.26	A.
	MOTA	1450	CB	LEU .	Α	254	48.858	37.006	20.564	1.00	25.84	A
	ATOM	1451	CG	LEU.	Α	254	47.882	36.290	19.621	1.00	24.69	A
	ATOM	1452	CD1	LEU .	Α	254	46.459	36.724	19.932	1.00	23.64	A
20	ATOM	1453	CD2	LEU .	Α	254	48.236	36.597	18.177	1.00	24.24	A
	ATOM	1454	С	LEU	Α	254	51.134	37.314	21.537	1.00	30.62	A
	ATOM	1455	0	LEU			51.633	38.383	21.187	1.00	32.35	A
	ATOM	1456	N	THR			51.292	36.821	22.758		32.47	A
	ATOM	1457	CA	THR			52.056	37.547	23.759		36.70	A
25	ATOM	1458	CB	THR			51.368	37.478	25.127		34.51	A
	ATOM	1459					51.188	36.106	25.494		35.49	A
	ATOM	1460					50.013	38.166	25.077		33.40	A
	ATOM	1461	C	THR			53.477	37.035	23.910		40.09	A
		1462	0	THR			54.430	37.793	23.772		43.69	A
30	ATOM ATOM	1463	N	GLU			53.617	35.747	24.189		44.77	A
30												
	ATOM	1464	CA	GLU .			54.932	35.144	24.382		49.15	A
	ATOM	1465	CB	GLU			54.866	34.143	25.534		51.24	A
	ATOM	1466	CG	GLU			54.514	34.786	26.862		56.03	A
	ATOM	1467	CD	GLU			54.053	33.780	27.893		58.83	A
35	MOTA	1468					54.766	32.776	28.107		62.13	A
	MOTA	1469		GLU			52.979	33.996	28.494		60.34	A
	MOTA	1470	С	GLU			55.475	34.456	23.137		50.09	A
	MOTA	1471	0	GLU			56.616	33.995	23.127		50.42	A
	MOTA	1472	N	LYS			54.658	34.389	22.090		51.21	A
40	MOTA	1473	CA	LYS			55.064	33.746	20.845		51.22	A
	MOTA	1474	CB	LYS			56.244	34.502	20.227		53.28	A
	MOTA	1475	CG	LYS			56.558	34.125	18.790	1.00	55.19	A
	MOTA	1476	CD	LYS	Α	257	57.709	34.961	18.253	1.00	57.52	A
	MOTA	1477	CE	LYS	Α	257	57.952	34.694	16.777	1.00	58.52	A
45	MOTA	1478	NZ	LYS	Α	257	58.290	33.268	16.515	1.00	60.88	A
	ATOM	1479	C	LYS	Α	257	55.467	32.302	21.138	1.00	50.74	A
	ATOM	1480	0	LYS	А	257	56.432	31.790	20.577	1.00	52.26	A
	ATOM	1481	N	SER	А	258	54.721	31.654	22.027	1.00	48.07	A
	ATOM	1482	CA	SER			54.999	30.273	22.402		46.87	A
50	ATOM	1483	CB	SER			55.590	30.229	23.812		48.88	A
	ATOM	1484	OG	SER			54.741	30.892	24.734		53.14	A
	ATOM	1485	C	SER			53.735	29.415	22.342		44.07	A
	ATOM	1486	0	SER			52.617	29.932	22.417		44.17	A
	ATOM	1487	N	ALA			53.917	28.105	22.204		38.30	A
55	MOTA	1488	CA				52.793		22.204		34.73	A A
33				ALA				27.180				
	MOTA	1489	CB	ALA			52.551	26.779	20.684		34.16	A
	MOTA	1490	C	ALA			53.042	25.940	22.977		32.34	A
	ATOM	1491	0	ALA			54.172	25.459	23.086		31.81	A
	MOTA	1492	N	CYS	A	260	51.975	25.428	23.579	1.00	28.58	A

	ATOM	1493	CA	CYS	Α	260	52.056	24.244	24.425	1.00 2	26.27	A
	ATOM	1494	CB	CYS	Α	260	52.183	24.654	25.892	1.00 2	26.53	A
	ATOM	1495	SG			260	50.846	25.739	26.469	1.00		A
	MOTA	1496	C	CYS	Α	260	50.786	23.435	24.224	1.00 2	22.83	A
5	ATOM	1497	0	CYS	А	260	49.892	23.856	23.495	1.00 2	22.14	A
	ATOM	1498	N			261	50,706	22.277	24.868	1.00 2		A
	ATOM	1499	CA			261	49.526	21.434	24.744	1.00 2		A
	ATOM	1500	CB	LYS	Α	261	49.619	20.243	25.696	1.00 2	23.28	A
	ATOM	1501	CG	LYS	A	261	50.716	19.253	25.347	1.00 2	27.44	A
10	ATOM	1502	CD	LYS			50.732	18.117	26.350	1.00		A
10												
	MOTA	1503	CE	LYS	Α	261	51.922	17.203	26.134	1.00	32.34	A
	ATOM	1504	NZ	LYS	A	261	51.940	16.121	27.153	1.00	33.28	A
	ATOM	1505	С	LYS	Δ	261	48.268	22.229	25.062	1.00	19 20	A
	ATOM	1506	ō	LYS			47.253	22.092	24.387	1.00		A
15	MOTA	1507	N			262	48.358	23.068	26.089	1.00		A
	ATOM	1508	CA	SER	Α	262	47.235	23.883	26.534	1.00	18.13	A.
	ATOM	1509	CB	SER	A	262	47.644	24.698	27,770	1.00	18.27	A
	ATOM	1510	OG			262	46.517	25.258	28.421	1.00		A
	MOTA	1511	C	SER	Α	262	46.736	24.811	25.424	1.00	16.77	A
20	ATOM	1512	0	SER	Α	262	45.591	25.254	25.450	1.00	L5.69	A
	ATOM	1513	N	SER	Δ	263	47.595	25.118	24.456	1.00	16 44	A
	MOTA	1514	CA			263	47.175	25.970	23.347	1.00		A
	MOTA	1515	CB	SER	Α	263	48.340	26.228	22.382	1.00	L8.49	A.
	ATOM	1516	OG	SER	Α	263	49.402	26.909	23.031	1.00 2	22.10	A
25	ATOM	1517	C			263	46.040	25.257	22.612	1.00		A
23												
	MOTA	1518	0			263	45.099	25.898	22.148	1.00		A
	ATOM	1519	N	ASP	A	264	46.119	23.928	22.517	1.00	16.30	A
	ATOM	1520	CA	ASP	A	264	45.069	23.166	21.836	1.00	16.72	A
	ATOM	1521	CB	ASP			45.483	21.704	21.620	1.00		A
20												
30	MOTA	1522	CG	ASP			46.544	21.539	20.548	1.00		A
	MOTA	1523	OD1	ASP	Α	264	46.642	22.412	19.661	1.00	L6.78	A.
	ATOM	1524	OD2	ASP	A	264	47.265	20.515	20.579	1.00	16.64	A
	ATOM	1525	C	ASP			43.773	23.194	22.646	1.00		A
	MOTA	1526	0	ASP			42.681	23.197	22.076	1.00		A
35	ATOM	1527	N	LEU	Α	265	43.898	23.205	23.974	1.00	15.49	A.
	ATOM	1528	CA	LEU			42.730	23.232	24.849	1.00	14 75	A
	ATOM	1529		LEU				23.038				
			CB				43.147		26.313	1.00		A
	MOTA	1530	CG	LEU	A	265	43.711	21.641	26.621	1.00	L4.04	A
	MOTA	1531	CD1	LEU	Α	265	44.249	21.579	28.052	1.00	13.96	A
40	ATOM	1532	CD2	LEU	Δ	265	42.619	20.603	26.416	1.00	11 62	A
	ATOM	1533	C			265	41.999	24.557	24.675	1.00		
												A
	MOTA	1534	0	LEU	Α	265	40.777	24.620	24.785	1.00	16.75	A
	MOTA	1535	N	TRP	A	266	42.746	25.622	24.405	1.00	L6.08	A
	ATOM	1536	CA	TRP	Δ	266	42.118	26.918	24.184	1.00	16 96	A
45												
45	MOTA	1537	CB			266	43.176	28.015	24.023	1.00		A
	MOTA	1538	CG	TRP	Α	266	42.618	29.326	23.521	1.00 2	20.54	A.
	ATOM	1539	CD2	TRP	Α	266	42.313	30.490	24.301	1.00 2	20.07	A
	ATOM	1540	CF2	TRP	Th.	266	41.782	31.459	23.417	1.00 2	20 46	A
	MOTA	1541		TRP			42.435	30.810	25.660	1.00 2		A
50	MOTA	1542	CD1	TRP	Α	266	42.270	29.631	22.231	1.00	L9.53	A
	ATOM	1543	NE1	TRP	Α	266	41.769	30.908	22.163	1.00	19.61	A
	ATOM	1544	CZ2	TRP			41.372	32.727	23.850	1.00		A
	ATOM	1545	CZ3				42.026	32.073	26.091	1.00		A
	ATOM	1546	CH2	TRP	Α	266	41.501	33.015	25.185	1.00 2	20.71	A
55	ATOM	1547	С	TRP	Α	266	41.284	26.795	22.913	1.00	17.22	A
	ATOM	1548	0			266	40.139	27.240	22.863	1.00		A
	MOTA	1549	N	ALA			41.863	26.181	21.886	1.00		A
	ATOM	1550	CA	ALA	Α	267	41.155	25.990	20.626	1.00	16.16	A
	ATOM	1551	CB	ALA	Α	267	42.050	25.290	19.621	1.00	L4.28	A

	3.0001	1550	~			0.67	-	0 001	05 150	00 001	1 00	16.00	
	MOTA	1552	C	ALA				9.901	25.159	20.891		16.28	A
	MOTA	1553	0	ALA	А	267	3	8.835	25.436	20.346	1.00	16.46	A
	ATOM	1554	N	LEU	Α	268	4	0.031	24.144	21.739	1.00	16.57	A
	ATOM	1555	CA	TEIL	75	268	3	8.890	23.299	22.084	1 00	17.03	A
5													
3	MOTA	1556	CB			268		9.292	22.260	23.139		15.35	A
	MOTA	1557	CG	LEU	Α	268	3	8.158	21.429	23.754		19.00	A
	ATOM	1558	CD1	LEU	Α	268	3	7.505	20.578	22.678	1.00	16.17	A
	ATOM	1559	CD2	LEU	А	268	3	8.718	20.537	24.881	1.00	17.49	A
	ATOM	1560	C			268		7.766	24.179	22.628		15.72	A
10													
10	MOTA	1561	0			268		6.603	24.031	22.247		15.28	A
	MOTA	1562	N			269		8.119	25.099	23.520		14.34	A
	ATOM	1563	CA	GLY	Α	269	3	7.124	25.989	24.092	1.00	13.39	A
	ATOM	1564	C	GLY	Α	269	3	6.406	26.808	23.031	1.00	14.94	A
	ATOM	1565	0			269		5.193	27.014	23.114	1 00	14.76	A
15	ATOM	1566	N			270		7.146	27.279	22.030		13.86	A
13													
	MOTA	1567	CA			270		6.539	28.061	20.958		16.80	A
	MOTA	1568	CB	CYS	Α	270	3	7.611	28.634	20.023	1.00	15.97	A
	ATOM	1569	SG	CYS	Α	270	3	8.751	29.810	20.780	1.00	20.48	A
	ATOM	1570	C	CYS	А	270	3	5.598	27.175	20.140	1.00	17.50	A
20	ATOM	1571	ō			270		4.516	27.604	19.741		18.38	A
20													
	MOTA	1572	N			271		6.022	25.939	19.887		16.99	A
	MOTA	1573	CA			271		5.221	25.004	19.104		16.66	A
	ATOM	1574	CB	ILE	Α	271	3	6.038	23.741	18.778	1.00	16.53	A
	ATOM	1575	CG2	ILE	Α	271	3	5.155	22.694	18.102	1.00	16.34	A
25	ATOM	1576		ILE				7.222	24.129	17.882		15.59	A
	ATOM	1577		ILE				8.239	23.018	17.690		14.88	A
	MOTA	1578	С			271		3.920	24.626	19.809		16.74	A
	ATOM	1579	0	ILE	Α	271	3	2.865	24.576	19.179		17.12	A
	ATOM	1580	N	ILE	Α	272	3	3.990	24.357	21.111	1.00	16.13	A
30	ATOM	1581	CA	ILE	Α	272	3	2.785	24.021	21.862	1.00	18.30	A
	ATOM	1582	CB			272		3.097	23.747	23.346		17.77	A
	ATOM	1583		ILE				1.796	23.666	24.152		17.96	A
	MOTA	1584		ILE				3.877	22.437	23.481		19.55	A
	MOTA	1585	CD1	ILE	Α	272	3	4.446	22.217	24.886	1.00	18.64	A
35	ATOM	1586	C	ILE	Α	272	3	1.824	25.207	21.776	1.00	19.51	A
	ATOM	1587	0	TLE	А	272		0.624	25.037	21.554	1.00	20.44	A
	ATOM	1588	N			273		2.362	26.409	21.947		18.52	A
	MOTA	1589	CA			273		1.553	27.615	21.881		20.48	A
	MOTA	1590	CB			273		2.418	28.847	22.162		18.98	A
40	MOTA	1591	CG	TYR	Α	273	3	1.663	30.161	22.125	1.00	20.26	A
	ATOM	1592	CD1	TYR	Α	273	3	1.229	30.709	20.916	1.00	20.67	A
	ATOM	1593	CE1	TYR	А	273	3	0.536	31.917	20.880	1.00	20.98	A
	ATOM	1594	CD2	TYR				1.383	30.857	23.302		19.82	A
	MOTA	1595		TYR				0.691	32.062	23.280		20.62	A
45	MOTA	1596	CZ			273		0.271	32.587	22.067		21.15	A
	MOTA	1597	OH	TYR	Α	273	2	9.588	33.776	22.049	1.00	21.86	A
	ATOM	1598	С	TYR	Α	273	3	0.902	27.730	20.507	1.00	21.54	A
	ATOM	1599	0	TYR	Δ	273	2	9.719	28.049	20.401	1 00	22.80	A
	ATOM	1600	N	GLN				1.676	27.454	19.461		21.05	A
50													
30	MOTA	1601	CA	GLN				1.176	27.538	18.095		21.48	A
	MOTA	1602	CB			274		2.323	27.341	17.097		21.41	A
	MOTA	1603	CG	GLN	Α	274	3	1.934	27.596	15.645	1.00	23.15	A
	ATOM	1604	CD	GLN	Α	274	3	3.131	27.588	14.706	1.00	24.80	A
	ATOM	1605		GLN				4.276	27.446	15.139		22.51	A
55	ATOM	1606		GLN					27.750			22.96	A
23								2.870		13.413			
	MOTA	1607	C			274		0.076	26.517	17.828		21.51	A
	MOTA	1608	0			274		9.123	26.806	17.108		20.50	A
	MOTA	1609	N	LEU	Α	275	3	0.207	25.324	18.403	1.00	21.44	A
	ATOM	1610	CA	LEU	Α	275	2	9.196	24.282	18.208	1.00	20.95	A

	ATOM	1611	CB	LEU	Α	275	29.645	22.958	18.846	1.00 19	.11	A
	ATOM	1612	CG	LEU	Α	275	30.775	22.182	18.159	1.00 21	.43	A
	ATOM	1613	CD1	LEU	Α	275	31.118	20.936	18.963	1.00 17	.64	A
	ATOM	1614	CD2	LEU	А	275	30.342	21.795	16.754	1.00 20	.34	A
5	ATOM	1615	С	LEH	А	275	27.860	24.697	18.815	1.00 21	. 32	A
	ATOM	1616	ō			275	26.802	24.461	18.229	1.00 19		A
	ATOM	1617	N			276	27.921	25.322	19.987	1.00 19		A
	ATOM	1618	CA	VAL			26.724	25.750	20.702	1.00 22		A
	ATOM	1619	CB			276	27.011	25.882	22.217	1.00 22		A
10				VAL								
10	MOTA	1620					25.742	26.291	22.957	1.00 19		A
	MOTA	1621		VAL			27.550	24.558	22.766	1.00 19		A
	ATOM	1622	C	VAL			26.127	27.075	20.211	1.00 23		A
	MOTA	1623	0			276	24.910	27.199	20.070	1.00 24		A
	MOTA	1624	N	ALA			26.983	28.062	19.965	1.00 24		A
15	MOTA	1625	CA	ALA			26.533	29.374	19.518	1.00 24		A
	ATOM	1626	CB	ALA			27.504	30.444	19.999	1.00 24		A
	MOTA	1627	C	ALA	Α	277	26.378	29.458	18.005	1.00 25	.76	A
	MOTA	1628	0	ALA	Α	277	25.577	30.242	17.502	1.00 26	.39	A
	ATOM	1629	N	GLY	Α	278	27.142	28.651	17.280	1.00 25	.13	A
20	ATOM	1630	CA	GLY	Α	278	27.062	28.673	15.834	1.00 25	.58	A.
	ATOM	1631	C	GLY	Α	278	28.163	29.524	15.231	1.00 26	.50	A
	ATOM	1632	0	GLY			28.374	29.510	14.015	1.00 28		A
	ATOM	1633	N	LEU	А	279	28.866	30.262	16.086	1.00 24	.44	A
	ATOM	1634	CA	LEU			29.962	31.130	15.656	1.00 25	. 21	A
25	ATOM	1635	CB	LEU			29.468	32.575	15.500	1.00 25		A
	ATOM	1636	CG	LEU			28.364	32.899	14.490	1.00 28		A
	ATOM	1637		LEU			27,922	34.344	14.684	1.00 26		A
	ATOM	1638		LEU			28.862	32.670	13.071	1.00 26		A
	ATOM	1639	C	LEU			31.093	31.116	16.687	1.00 23		A
30	ATOM	1640	Ö	LEU		279	30.848	30.994	17.882	1.00 24		A
30	ATOM	1641	N			280	32.349	31.239	16.236	1.00 23		A
	ATOM	1642	CD			280	32.831	31.404	14.855	1.00 22		A
	ATOM	1643	CA			280	33.464	31.239	17.189	1.00 23		A
	MOTA	1644	CB			280	34.692	31.293	16.282	1.00 23		A
35	MOTA	1645	CG			280	34.189	32.020	15.073	1.00 24		A
	MOTA	1646	C			280	33.353	32.444	18.137	1.00 22		A
	MOTA	1647	0			280	32.750	33.457	17.788	1.00 22		A
	MOTA	1648	N			281	33.939	32.344	19.345	1.00 23		A
	MOTA	1649	CD			281	34.810	31.223	19.734	1.00 21		A
40	MOTA	1650	CA			281	33.935	33.375	20.395	1.00 23		A
	MOTA	1651	CB	PRO	Α	281	34.781	32.751	21.509	1.00 24	.89	A.
	MOTA	1652	CG	PRO	Α	281	34.749	31.287	21.219	1.00 25	.24	A
	ATOM	1653	C	PRO	Α	281	34.481	34.752	20.017	1.00 23	.75	A
	MOTA	1654	0	PRO	Α	281	33.869	35.781	20.317	1.00 21	.02	A
45	ATOM	1655	N	PHE	Α	282	35.644	34.763	19.379	1.00 22	.17	A
	ATOM	1656	CA	PHE	А	282	36.293	36.007	18.998	1.00 23	.16	A
	ATOM	1657	CB			282	37.765	35.943	19.406	1.00 21		A
	ATOM	1658	CG			282	37.975	35.482	20.822	1.00 22		A
	ATOM	1659		PHE			37.806	36.361	21.888	1.00 20		A
50	ATOM	1660		PHE			38.291	34.151	21.093	1.00 20		A
50	ATOM	1661	CE1	PHE			37.947	35.921	23.206	1.00 22		A
	ATOM	1662		PHE			38.433	33.702	22.405	1.00 22		A
	ATOM	1663	CZ			282	38.261	34.590	23.466	1.00 20		A
	ATOM	1664	C			282	36.169	36.263	17.503	1.00 24		A
55	MOTA	1665	0			282	36.802	35.585	16.694	1.00 25		A
	MOTA	1666	N	ARG			35.355	37.248	17.142	1.00 24		A
	ATOM	1667	CA	ARG			35.141	37.594	15.741	1.00 26		A
	MOTA	1668	CB	ARG			33.721	37.209	15.316	1.00 28		A
	MOTA	1669	CG	ARG	Α	283	33.293	35.808	15.724	1.00 30	.27	A

	ATOM	1670	CD	ARG	Α	283	31.904	35.493	15.188	1.00	33.36	A
	MOTA	1671	NE	ARG	А	283	30.890	36.392	15.733	1.00	32.76	A
	ATOM	1672	CZ			283	30.372	36.287	16.952		34.79	A
	MOTA	1673		ARG			30.767	35.317	17.768		35.77	A
5	MOTA	1674		ARG			29.458	37.156	17.359		36.12	A
	MOTA	1675	C	ARG	Α	283	35.328	39.096	15.544	1.00	26.47	A
	ATOM	1676	0	ARG	Α	283	35.029	39.888	16.438	1.00	26.28	A
	ATOM	1677	N	ALA	A	284	35.818	39.486	14.373	1.00	26.70	A
	ATOM	1678	CA	ALA			36.033	40.899	14.079		27.84	A
10	ATOM	1679	CB	ALA			37.188	41.442	14.914		26.24	A
10	ATOM	1680	C			284	36.327	41.077	12.602		28.35	A
	MOTA	1681	0	ALA			36.560	40.101	11.891		29.91	A
	MOTA	1682	N			285	36.332	42.329	12.153		29.29	A
	ATOM	1683	CA	GLY	Α	285	36.577	42.631	10.753	1.00	29.52	A
15	ATOM	1684	C	GLY	Α	285	37.893	42.156	10.168	1.00	30.12	A
	ATOM	1685	0	GLY	Α	285	37.974	41.862	8.976	1.00	30.60	A
	ATOM	1686	N	ASN	А	286	38,939	42.097	10.983	1.00	28.49	A
	ATOM	1687	CA			286	40.231	41.644	10.489		26.71	A
	ATOM	1688	CB			286	41.050	42.825	9.945		26.11	A
20												
20	ATOM	1689	CG			286	41.310	43.900	10.990		27.83	A
	MOTA	1690		ASN			41.877	43.631	12.049		27.84	A
	MOTA	1691	ND2	ASN			40.908	45.131	10.685		25.95	A
	ATOM	1692	C	ASN	Α	286	40.997	40.924	11.584	1.00	26.03	A
	MOTA	1693	0	ASN	Α	286	40.540	40.851	12.723	1.00	25.66	A
25	ATOM	1694	N	GLU	Α	287	42.162	40.391	11.239	1.00	24.81	A
	ATOM	1695	CA			287	42.965	39.662	12.206		27.59	A
	ATOM	1696	CB			287	44.145	38.985	11.510		30.17	A
	ATOM	1697	CG			287	43.776	37.632	10.931		38.21	A
						287						
20	ATOM	1698	CD				44.900	36.998	10.140		41.86	A
30	MOTA	1699		GLU			46.061	37.036	10.608		43.08	A
	MOTA	1700	OE2	GLU			44.612	36.449	9.052		45.22	A
	ATOM	1701	С	GLU	Α	287	43.459	40.485	13.383	1.00	25.05	A
	MOTA	1702	0	GLU	Α	287	43.382	40.030	14.521	1.00	26.41	A
	ATOM	1703	N	TYR	Α	288	43.966	41.685	13.122	1.00	23.04	A
35	ATOM	1704	CA	TYR	А	288	44.460	42.528	14.205	1.00	22.34	A
	ATOM	1705	CB			288	44.867	43.913	13.691		21.07	A
	ATOM	1706	CG			288	45.275	44.858	14.805		21.07	A
	ATOM	1707		TYR			46.533	44.762	15.405		21.23	A
	MOTA	1708		TYR			46.891	45.588	16.475		20.43	A
40	MOTA	1709		TYR			44.380	45.809	15.302		22.32	A
	MOTA	1710	CE2				44.725	46.637	16.373		23.28	A
	MOTA	1711	CZ			288	45.981	46.518	16.953	1.00	22.96	A
	ATOM	1712	OH	TYR	Α	288	46.316	47.313	18.024	1.00	23.18	A
	ATOM	1713	C	TYR	Α	288	43.402	42.698	15.288	1.00	21.38	A
45	ATOM	1714	0	TYR	А	288	43.710	42.616	16.473	1.00	22.09	A
	ATOM	1715	N			289	42.159	42.939	14.874		21.88	A
	ATOM	1716	CA			289	41.055	43.130	15.811		21.98	A
	ATOM	1717	CB			289	39.821	43.673	15.078		22.90	A
	MOTA	1718	CG			289	39.896	45.130	14.601		26.52	A
50	MOTA	1719		LEU			38.706	45.436	13.696		26.55	A
	MOTA	1720	CD2	LEU	Α	289	39.914	46.071	15.807	1.00	23.13	A
	MOTA	1721	C	LEU	Α	289	40.686	41.849	16.560	1.00	21.24	A
	ATOM	1722	0	LEU	Α	289	40.256	41.897	17.715	1.00	20.72	A
	ATOM	1723	N			290	40.843	40.708	15.900		19.62	A
55	ATOM	1724	CA			290	40.538	39.433	16.533		18.54	A
	ATOM	1725	CB			290	40.560	38.281	15.509		18.52	A
	ATOM	1726		ILE			40.503	36.934	16.234		17.63	A
	ATOM	1727		ILE			39.378	38.429	14.545		18.88	A
	ATOM	1728	CD1	ILE	Α	290	39.421	37.483	13.357	1.00	19.81	A

	ATOM	1729	C	ILE A	290	41.578	39.167	17.618	1 00	19.09	A
	ATOM	1730	Ö	ILE A				18.737		18.20	A
	ATOM	1731	N	PHE 2				17.286		18.76	A
-	ATOM	1732	CA	PHE 2				18.247		20.75	A
5	ATOM	1733	CB	PHE A				17.606		20.71	A
	MOTA	1734	CG	PHE A				16.503		22.92	A
	ATOM	1735		PHE 2				16.443		22.98	A
	ATOM	1736	CD2					15.543		22.91	A
	ATOM	1737		PHE A				15.440		24.51	A
10	MOTA	1738		PHE A				14.535		25.54	A.
	MOTA	1739	CZ	PHE A	291	. 46.370	36.670	14.485	1.00	23.29	A
	ATOM	1740	С	PHE 2	291	. 43.739	40.061	19.451	1.00	21.72	A
	ATOM	1741	0	PHE A	291	43.992	39.671	20.593	1.00	22.32	A
	ATOM	1742	N	GLN A	292	43.284	41.275	19.178	1.00	23.27	A
15	ATOM	1743	CA	GLN A	292	43.055	42.264	20.216	1.00	24.01	A
	ATOM	1744	CB	GLN A	292	42.574	43.559	19.562	1.00	25.77	A
	ATOM	1745	CG	GLN A	292	42.57	44.773	20.447	1.00	28.45	A
	ATOM	1746	CD	GLN A				19.638		29.83	A
	ATOM	1747		GLN A				18.872		27.16	A
20	ATOM	1748	NE2	GLN A				19.799		27.61	A
20	ATOM	1749	C	GLN A				21.204		22.97	A
	ATOM	1750	Ö	GLN A				22.415		21.64	A
	ATOM	1751	N	LYS A				20.687		21.82	A
								21.558			
25	ATOM	1752	CA	LYS A						22.18	A
23	ATOM	1753	CB	LYS A				20.740		22.69	A
	ATOM	1754	CG	LYS A				20.153		25.78	A
	ATOM	1755	CD	LYS A				19.429		27.88	A
	ATOM	1756	CE	LYS A				18.926		30.85	A
	MOTA	1757	NZ	LYS A				18.214		32.98	A
30	ATOM	1758	C	LYS A				22.343		21.20	A
	ATOM	1759	0	LYS A				23.509		22.01	A
	ATOM	1760	N	ILE A				21.702		19.91	A
	MOTA	1761	CA	ILE A				22.347		20.28	A
	ATOM	1762	CB	ILE A				21.349		18.98	A
35	ATOM	1763	CG2	ILE A	294	43.483	1 35.550	22.098	1.00	17.70	A
	ATOM	1764	CG1	ILE A	294	41.716	35.897	20.318	1.00	17.93	A
	ATOM	1765	CD1	ILE A	294	42.46	7 35.237	19.178	1.00	16.21	A
	MOTA	1766	С	ILE A	294	42.618	37.727	23.587	1.00	21.94	A
	ATOM	1767	0	ILE A	294	42.366	37.199	24.673	1.00	20.86	A
40	ATOM	1768	N	ILE A	295	43.610	38.600	23.439	1.00	21.88	A
	ATOM	1769	CA	ILE A	295	44.46	L 38.934	24.582	1.00	24.25	A
	ATOM	1770	CB	ILE A	295	45.668	39.805	24.175	1.00	23.93	A
	ATOM	1771	CG2	ILE A	295	46.51	39.066	23.140	1.00	24.61	A
	ATOM	1772		ILE A				23.637		24.58	A
45	ATOM	1773		ILE A				23.433		26.69	A
	ATOM	1774	C	ILE A				25.717		24.80	A
	ATOM	1775	o	ILE A				26.842		24.76	A
	ATOM	1776	N	LYS A				25.425		25.33	A
	ATOM	1777	CA	LYS A				26.444		26.80	A
50	ATOM	1778	CB	LYS A				25.894		27.39	A
50											
	MOTA	1779	CG	LYS A				25.413		31.79	A
	ATOM	1780	CD	LYS A				24.826		35.56	A
	ATOM	1781	CE	LYS A				25.900		39.29	A
	ATOM	1782	NZ	LYS A				25.357		41.72	A
55	MOTA	1783	C	LYS A				26.893		25.50	A
	MOTA	1784	0	LYS A				27.713		24.02	A
	MOTA	1785	N	LEU A				26.349		25.67	A
	MOTA	1786	CA	LEU A				26.666		25.16	A
	MOTA	1787	CB	LEU A	297	39.632	37.285	28.111	1.00	24.80	A

	ATOM	1788	CG	LEU	А	297	38.766	36.068	28.460	1.00	26.43	A
	ATOM	1789		LEU			39.238	34.852	27.646		26.70	A
	ATOM	1790		LEU			38.856	35.777	29.951		24.84	A
	ATOM	1791	C	LEU			38.151	38.459	26.467		25.11	A
5	ATOM	1792	ō	LEU			37.261	38.378	27.309		25.28	A
,	ATOM	1793	N	GLU			38.007	39.127	25.331		24.98	A
	ATOM	1794	CA	GLU			36.786				25.31	
								39.847	25.023			A
	ATOM	1795	CB	GLU			37.143	41.139	24.291		27.13	A
	MOTA	1796	CG	GLU			35.991	42.092	24.108		31.28	A
10	MOTA	1797	CD	GLU			36.419	43.362	23.410		34.40	A
	MOTA	1798		GLU			37.348	44.027	23.918		35.90	A
	ATOM	1799		GLU			35.832	43.693	22.359		36.16	A
	MOTA	1800	С	GLU			35.766	39.057	24.207		23.79	A
	ATOM	1801	0	GLU	Α	298	35.832	39.017	22.979	1.00	24.35	A
15	MOTA	1802	N	TYR	Α	299	34.825	38.427	24.902	1.00	23.45	A
	ATOM	1803	CA	TYR	Α	299	33.760	37.663	24.265	1.00	23.98	A
	ATOM	1804	CB	TYR	Α	299	34.264	36.304	23.755	1.00	20.13	A
	ATOM	1805	CG	TYR	Α	299	34.348	35.233	24.828	1.00	21.17	A
	ATOM	1806	CD1	TYR	Α	299	35.336	35.279	25.810	1.00	19.32	A
20	ATOM	1807	CE1	TYR	Α	299	35.389	34.332	26.826	1.00	19.30	A
	ATOM	1808	CD2	TYR	Α	299	33.410	34.201	24.888	1.00	18.96	A
	ATOM	1809	CE2	TYR	А	299	33.456	33.243	25.907	1.00	19.41	A
	ATOM	1810	CZ			299	34.449	33.321	26.870		18.79	A
	ATOM	1811	OH	TYR			34.511	32.401	27.881		18.77	A
25	ATOM	1812	C			299	32.699	37.437	25.331		25.20	A
	ATOM	1813	ō	TYR			32.942	37.681	26.506		26.46	A
	ATOM	1814	N	ASP			31.522	36.981	24.927		26.94	A
	ATOM	1815	CA	ASP			30.467	36.710	25.891		30.60	A
	ATOM	1816	CB	ASP			29.665	37.981	26.179		35.86	A
30	ATOM	1817	CG	ASP			29.228	38.687	24.923		42.04	A
30	ATOM			ASP			28.450	38.088	24.923		45.98	
		1818										A
	ATOM	1819		ASP			29.666	39.840	24.707		45.69	A
	MOTA	1820	С	ASP			29.564	35.608	25.363		29.26	A
	MOTA	1821	0	ASP			29.590	35.299	24.172		28.64	A
35	ATOM	1822	N	PHE			28.778	35.011	26.253		28.96	A
	ATOM	1823	CA	PHE			27.884	33.924	25.871		30.48	A
	MOTA	1824	CB	PHE			27.818	32.854	26.968		29.17	A
	MOTA	1825	CG	PHE			29.147	32.279	27.356		29.29	A
	MOTA	1826		PHE			29.978	32.949	28.245		27.31	A
40	MOTA	1827					29.560	31.050	26.845		27.89	A
	MOTA	1828		PHE			31.205	32.403	28.625		28.83	A
	MOTA	1829	CE2				30.781	30.498	27.217		28.05	A
	MOTA	1830	CZ	PHE	Α	301	31.605	31.175	28.110	1.00	28.27	A
	MOTA	1831	C	PHE	Α	301	26.459	34.384	25.619	1.00	32.20	A
45	ATOM	1832	0	PHE	Α	301	25.946	35.261	26.317	1.00	32.36	A
	ATOM	1833	N	PRO	Α	302	25.798	33.804	24.607	1.00	33.29	A
	ATOM	1834	CD	PRO	Α	302	26.313	32.943	23.529	1.00	34.04	A
	ATOM	1835	CA	PRO	Α	302	24.415	34.199	24.341	1.00	35.24	A
	MOTA	1836	CB	PRO			24.144	33.608	22.959		34.01	A
50	ATOM	1837	CG	PRO			25.041	32.413	22.921		35.48	A
	ATOM	1838	C	PRO			23.567	33.561	25.444		37.39	A
	ATOM	1839	ō	PRO			23.935	32.518	25.986		38.49	A
	ATOM	1840	N	ALA			22.447	34.188	25.783		39.36	A
	ATOM	1841	CA	ALA			21.572	33.692	26.843		40.65	A
55	ATOM	1842	CB	ALA			20.280	34.506	26.862		41.66	A
22	ATOM	1843	С	ALA			21.238	32.197	26.814		41.25	A
	ATOM	1844	Ö	ALA			21.253	31.537	27.854		43.16	A
	ATOM	1845	N	ALA			20.945	31.665	25.631		41.04	A
		1845	N CA	ALA							40.66	
	MOTA	1846	CA	АЬА	А	JU4	20.569	30.258	25.480	1.00	40.06	A

	7.00	1047	CD	ALA	20	204	20.121	30.004	24.040	1.00 41.36	70
	MOTA	1847	CB								A
	MOTA	1848	C	ALA	А	304	21.628	29.223	25.876	1.00 39.61	A
	ATOM	1849	0	ALA	Α	304	21.298	28.156	26.395	1.00 40.61	A
	ATOM	1850	N	PHE	Δ	305	22.891	29.543	25.617	1.00 36.21	A
5											
3	MOTA	1851	CA			305	24.022	28.662	25.909	1.00 32.08	A
	MOTA	1852	CB	PHE	Α	305	25.259	29.519	26.187	1.00 29.46	A
	ATOM	1853	CG	PHE	А	305	26.536	28.917	25.690	1.00 28.15	A
	ATOM	1854	CD1	PHE	Δ	305	27.146	27.875	26.377	1.00 26.20	A
	ATOM	1855	CD2				27.127	29.386	24.521	1.00 27.05	A
10	MOTA	1856					28.330	27.308	25.908	1.00 26.92	A
	MOTA	1857	CE2	PHE	Α	305	28.312	28.826	24.042	1.00 26.62	A
	ATOM	1858	CZ	PHE	Α	305	28.914	27.786	24.737	1.00 26.61	A
	MOTA	1859	C	PHE	Α	305	23.811	27.664	27.057	1.00 30.09	A
	ATOM	1860	0	PHE	Δ	305	23.518	28.051	28.187	1.00 31.51	A
15	ATOM	1861	N			306	23.964	26.378	26.758	1.00 27.01	A
13											
	ATOM	1862	CA			306	23.801	25.334	27.769	1.00 26.30	A
	MOTA	1863	CB			306	24.157	23.970	27.170	1.00 25.03	A
	MOTA	1864	CG	PHE	Α	306	23.548	23.725	25.815	1.00 27.24	A
	ATOM	1865	CD1	PHE	Α	306	22.170	23.831	25.622	1.00 28.40	A
20	ATOM	1866	CD2	PHE			24.350	23.386	24.728	1.00 27.84	A
20	ATOM	1867	CE1				21.601	23.603	24.365	1.00 28.05	A
	MOTA	1868	CE2			306	23.792	23.155	23.465	1.00 28.31	A
	ATOM	1869	CZ	PHE	Α	306	22.415	23.263	23.283	1.00 28.00	A
	MOTA	1870	C	PHE	Α	306	24.711	25.652	28.961	1.00 26.23	A.
25	ATOM	1871	0	PHE	А	306	25.927	25.775	28.811	1.00 25.59	A
	ATOM	1872	N			307	24.125	25.796	30.163	1.00 26.67	A
		1873				307				1.00 27.95	
	ATOM		CD				22.685	25.625	30.430		A
	MOTA	1874	CA			307	24.842	26.110	31.405	1.00 26.59	A
	MOTA	1875	CB	PRO	Α	307	23.795	25.832	32.481	1.00 26.14	A
30	ATOM	1876	CG	PRO	Α	307	22.531	26.250	31.803	1.00 27.86	A
	ATOM	1877	С	PRO	А	307	26.145	25.355	31.659	1.00 25.58	A
	ATOM	1878	ō			307	27.189	25.964	31.900	1.00 22.65	A
	MOTA	1879	N			308	26.085	24.031	31.620	1.00 24.46	A
	MOTA	1880	CA			308	27.274	23.232	31.867	1.00 23.91	A
35	ATOM	1881	CB	LYS	Α	308	26.887	21.760	32.024	1.00 23.25	A
	ATOM	1882	CG	LYS	Α	308	26.062	21.532	33.285	1.00 28.49	A
	ATOM	1883	CD	LYS	Δ	308	25.618	20.093	33.466	1.00 30.17	A
	ATOM	1884	CE			308	24.760	19.973	34.722	1.00 33.12	A
	MOTA	1885	NZ	LYS			24.122	18.636	34.860	1.00 34.13	A
40	MOTA	1886	C	LYS			28.314	23.426	30.769	1.00 22.84	A
	MOTA	1887	0	LYS	Α	308	29.514	23.411	31.042	1.00 22.46	A
	ATOM	1888	N	ALA	Α	309	27.861	23,621	29.534	1.00 21.59	A
	ATOM	1889	CA	ALA	А	309	28.792	23.848	28.432	1.00 20.02	A
	ATOM	1890	CB	ALA			28.056	23.856	27.106	1.00 18.80	A
45											
45	MOTA	1891	С	ALA			29.481	25.191	28.662	1.00 21.41	A
	MOTA	1892	0	ALA	Α	309	30.680	25.335	28.427	1.00 21.39	A
	MOTA	1893	N	ARG	Α	310	28.717	26.179	29.121	1.00 21.39	A
	ATOM	1894	CA	ARG	Α	310	29.290	27.494	29.388	1.00 22.02	A
	ATOM	1895	CB	ARG			28.213	28.479	29.854	1.00 22.39	A
50	ATOM	1896	CG	ARG			28.806	29.756	30.436	1.00 25.30	A
50											
	MOTA	1897	CD	ARG			27.780	30.852	30.664	1.00 28.33	A
	MOTA	1898	NE	ARG			28.420	32.039	31.230	1.00 30.18	A
	MOTA	1899	CZ	ARG	Α	310	27.901	33.263	31.203	1.00 32.07	A
	ATOM	1900	NH1	ARG	Α	310	26.719	33.477	30.634	1.00 31.19	A
55	ATOM	1901		ARG			28.567	34.277	31.742	1.00 30.49	A
	ATOM	1902	C	ARG			30.376	27.388	30.458	1.00 21.65	A
	MOTA	1903	0	ARG			31.464	27.949	30.311	1.00 20.36	A
	MOTA	1904	N	ASP			30.074	26.677	31.541	1.00 19.57	A
	ATOM	1905	CA	7 C D	70	311	31.043	26.512	32.615	1.00 20.18	A

	ATOM	1906	CB	ASP	Α	311	30.460	25.649	33.739	1.00	20.39	A
	ATOM	1907	CG	ASP	70	211	31.439	25.446	34.881	1 00	23.35	A
	MOTA	1908		ASP			32.158	24.428	34.885		24.91	A
	ATOM	1909	OD2	ASP	Α	311	31.500	26.312	35.776	1.00	26.96	A
5	ATOM	1910	С	ASP	А	311	32.322	25.877	32.073	1.00	19.73	A
	MOTA	1911	ō	ASP			33.422	26.289	32,439		19.30	A
	ATOM	1912	N	LEU	Α	312	32.179	24.891	31.188	1.00	16.32	A
	ATOM	1913	CA	LEU	Α	312	33.349	24.226	30.611	1.00	16.66	A
	ATOM	1914	CB	LEU	Δ	312	32.927	23.035	29.744	1 00	16.12	A
10	ATOM	1915	CG	LEU			34.050	22.320	28.974		14.73	A
10												
	MOTA	1916		LEU			35.192	21.935	29.912	1.00	14.56	A.
	ATOM	1917	CD2	LEU	Α	312	33.477	21.084	28.289	1.00	14.22	A
	ATOM	1918	С	LEU			34.181	25.189	29.774		16.61	A
	ATOM	1919	ō	LEU			35.402	25.241	29.910		16.20	A
15	MOTA	1920	N	VAL			33.515	25.949	28.908		16.20	A
	ATOM	1921	CA	VAL	Α	313	34.207	26.907	28.058	1.00	15.37	A
	ATOM	1922	CB	VAL	Δ	313	33,216	27.648	27,130	1.00	16.42	A
	MOTA	1923		VAL			33.915	28.796	26.426		16.93	A
	ATOM	1924	CG2	VAL	Α	313	32.644	26.672	26.103	1.00	17.88	A
20	ATOM	1925	C	VAL	Α	313	34.960	27.923	28.911	1.00	17.39	A
	ATOM	1926	ò			313	36.093	28.294	28.591		18.00	A
	MOTA	1927	N	GLU			34.342	28.364	30.004		17.61	A
	ATOM	1928	CA	GLU	Α	314	34.986	29.331	30.885	1.00	20.43	A
	ATOM	1929	CB	GLU	А	314	34.009	29.816	31.959	1.00	22.14	A
25	ATOM	1930	CG	GLU			32.800	30.550	31.396		26.52	A
23												
	MOTA	1931	CD	GLU			31.852	31.025	32.478		31.26	A
	ATOM	1932	OE1	GLU	Α	314	31.580	30.246	33.417	1.00	33.48	A
	MOTA	1933	OE2	GLU	Α	314	31.370	32.173	32.387	1.00	34.81	A
	ATOM	1934	С	GLU			36.217	28.721	31.539		19.15	Α
20												
30	MOTA	1935	0	GLU			37.134	29.433	31.934		21.47	A
	ATOM	1936	N	LYS	Α	315	36.245	27.400	31.651	1.00	19.51	A
	ATOM	1937	CA	LYS	А	315	37.394	26.749	32.258	1.00	19.17	A
	ATOM	1938	CB	LYS			36.946	25.514	33.043		18.84	A
	MOTA	1939	CG	LYS			36.280	25.885	34.368		19.62	A
35	ATOM	1940	CD	LYS	Α	315	35.653	24.696	35.073	1.00	19.22	A
	ATOM	1941	CE	LYS	А	315	35.070	25.095	36.427	1.00	21.00	A
	ATOM	1942	NZ	LYS			36.119	25.552	37.381		19.53	A
								26.393			18.96	
	MOTA	1943	С	LYS			38.452		31.218			A
	MOTA	1944	0	LYS	A	315	39.511	25.873	31.561	1.00	19.85	A
40	ATOM	1945	N	LEU	Α	316	38.164	26.691	29.950	1.00	17.08	A
	ATOM	1946	CA	T.RII	Δ	316	39.102	26.429	28.854	1 00	16.41	A
	ATOM	1947	CB	LEU			38.414	25.636	27.738		13.81	A
	ATOM	1948	CG			316	38.028	24.201	28.115		14.39	A.
	ATOM	1949	CD1	LEU	Α	316	37.139	23.597	27.031	1.00	12.38	A
45	MOTA	1950	CD2	LEU	А	316	39.302	23.373	28.309	1.00	12.77	A
	ATOM	1951	C			316	39.652	27.743	28.290		17.12	A
	MOTA	1952	0			316	40.851	27.860	28.023		16.53	A.
	ATOM	1953	N	LEU	A	317	38.780	28.729	28.105	1.00	16.27	A
	MOTA	1954	CA	LEU	Δ	317	39.228	30.022	27.596	1 00	17.52	A
50	ATOM	1955	CB	LEU			38.083	30.752	26.887		16.37	A
50												
	MOTA	1956	CG	LEU			37.448	29.973	25.727		18.81	A
	MOTA	1957	CD1	LEU	Α	317	36.415	30.851	25.018	1.00	16.47	A.
	ATOM	1958		LEU			38.528	29.526	24.741		17.87	A
	ATOM	1959	C	LEU			39.745	30.841	28.774		18.27	A
55	MOTA	1960	0	LEU			39.078	31.753	29.273		18.58	A
	ATOM	1961	N	VAL	Α	318	40.937	30.475	29.229	1.00	18.02	A
	MOTA	1962	CA	VAL	Α	318	41.593	31.141	30.342	1.00	18.85	A
	ATOM	1963	CB	VAL			41.846	30.153	31.500		19.91	A
	MOTA	1964	CGI	VAL	Α	310	42.590	30.848	32.634	1.00	20.01	A

	ATOM	1965	CG2	VAL	Α	318	40.520	29.584	31.990		19.44	A
	MOTA	1966	C	VAL			42.923	31.657	29.811		19.67	A
	MOTA	1967	0	VAL			43.690	30.902	29.208		18.26	A
	ATOM	1968	N	LEU	Α	319	43.197	32.939	30.028	1.00	20.07	A
5	ATOM	1969	CA	LEU	Α	319	44.436	33.533	29.538	1.00	20.98	A
	MOTA	1970	CB	LEU	Α	319	44.521	35.002	29.968		21.64	A
	ATOM	1971	CG	LEU			43.418	35.908	29.408		24.38	A
	ATOM	1972	CD1	LEU	Α	319	43.606	37.332	29.935	1.00	23.28	A
	ATOM	1973	CD2	LEU			43.453	35.887	27.875	1.00	24.33	A
10	ATOM	1974	C	LEU	Α	319	45.680	32.774	29.994	1.00	20.38	A
	MOTA	1975	0	LEU	Α	319	46.568	32.496	29.192	1.00	21.34	A
	ATOM	1976	N	ASP			45.742	32.440	31.280		20.22	A
	MOTA	1977	CA	ASP			46.879	31.707	31.833	1.00	20.90	A
	ATOM	1978	CB	ASP			46.842	31.760	33.365		20.76	A
15	MOTA	1979	CG	ASP			48.049	31.102	34.004		21.51	A
	ATOM	1980		ASP			48.669	30.226	33.367		23.46	A
	ATOM	1981	OD2	ASP			48.371	31.450	35.159		23.89	A
	MOTA	1982	C	ASP			46.814	30.247	31.367		20.06	A
	MOTA	1983	0	ASP			45.988	29.476	31.840		20.54	A
20	MOTA	1984	N	ALA			47.700	29.876	30.451		20.68	A
	MOTA	1985	CA	ALA			47.733	28.522	29.903		22.04	A
	MOTA	1986	CB	ALA			48.860	28.411	28.881		20.75	A
	MOTA	1987	C	ALA			47.858	27.400	30.940		21.62	A
	MOTA	1988	0	ALA			47.482	26.259	30.665		21.99	A
25	ATOM	1989	N	THR			48.372	27.715	32.127		20.89	A
	MOTA	1990	CA	THR			48.531	26.698	33.167		20.82	A
	MOTA	1991	CB	THR			49.670	27.051	34.146		19.47	A
	MOTA	1992		THR			49.341	28.253	34.848		20.19	A
	MOTA	1993		THR			50.981	27.249	33.394		21.59	A
30	MOTA	1994	C	THR			47.264	26.498	33.983		19.55	A
	MOTA	1995	0	THR			47.235	25.673	34.894		21.13	A
	MOTA	1996	N			323	46.216	27.248	33.661		19.33	A
	MOTA	1997	CA	LYS			44.962	27.122	34.392		21.20	A
	MOTA	1998	CB	LYS			44.580	28.460	35.030		23.75	A
35	MOTA	1999	CG	LYS			45.562	28.933	36.084		28.45	A
	ATOM	2000	CD	LYS			45.055	30.177	36.799		33.76	A
	MOTA	2001	CE	LYS			46.087	30.678	37.802		36.15	A
	MOTA	2002	NZ	LYS			46.532	29.569	38.693		37.34	A
40	MOTA	2003	C	LYS			43.806	26.614	33.539		20.68	A
40	ATOM	2004	0	LYS			42.649	26.757	33.915		20.42	A
	ATOM	2005	N	ARG			44.114	26.019	32.392		19.97	A
	ATOM	2006	CA	ARG			43.060	25.494	31.531		17.98	A
	ATOM	2007	CB	ARG			43.461	25.609	30.061		15.95	A
45	ATOM	2008	CG	ARG			43.534	27.050	29.603		17.34	A
45	ATOM	2009	CD	ARG			43.996	27.194	28.172		19.80	A
	ATOM	2010	NE	ARG			44.438	28.565	27.944		16.93	A
	ATOM	2011	CZ	ARG			45.410	28.908	27.108		19.88	A
	MOTA	2012		ARG			46.045	27.978	26.398		14.58	A
50	ATOM	2013		ARG			45.774	30.181	27.015		16.51	A
50	ATOM	2014	С	ARG			42.762	24.046	31.883		18.32	A
	ATOM	2015	0	ARG			43.673	23.222	32.006		18.20	A
	ATOM	2016	N	LEU			41.479	23.748	32.055		18.32	A
	ATOM	2017	CA	LEU			41.050	22.403	32.395		17.79	A
	ATOM	2018	CB	LEU			39.523	22.335	32.425		17.03	A
55	ATOM	2019	CG	LEU			38.896	21.125	33.116		15.91	A
	ATOM	2020		LEU			39.392	21.048	34.557		15.93	A
	ATOM	2021		LEU			37.375	21.255	33.084		16.56	A
	ATOM	2022	С			325	41.599	21.433	31.356		18.68	A
	ATOM	2023	0	LEU	Α	325	41.347	21.586	30.157	1.00	18.28	A

	ATOM	2024	N	GLY	Δ	326	42.354	20.439	31.821	1.00	18.18	A
	ATOM	2025	CA	GLY			42.931	19.462	30.915		16.36	A
	ATOM	2026	C	GLY			44.443	19.558	30.807		19.15	A
-	ATOM	2027	0	GLY			45.093	18.592	30.404		19.52	A
5	MOTA	2028	N	CYS			45.016	20.708	31.161		18.16	A
	MOTA	2029	CA	CYS			46.463	20.867	31.075		19.30	A
	ATOM	2030	CB	CYS			46.856	22.350	31.058		20.22	A
	MOTA	2031	SG	CYS			46.782	23.200	32.649		21.97	A
	MOTA	2032	C	CYS	Α	327	47.169	20.157	32.228	1.00	20.22	A
10	ATOM	2033	0	CYS	Α	327	46.561	19.828	33.246	1.00	17.92	A
	ATOM	2034	N	GLU	Α	328	48.463	19.933	32.053	1.00	20.51	A
	ATOM	2035	CA	GLU	Α	328	49.274	19.244	33.042	1.00	23.34	A
	ATOM	2036	CB	GLU	Α	328	50.710	19.139	32.507	1.00	28.68	A
	ATOM	2037	CG	GLU	Α	328	50.754	18.367	31.175	1.00	38.24	A
15	ATOM	2038	CD	GLU			52.067	18.500	30.414		43.23	A
	ATOM	2039		GLU			52.535	19.643	30.218		46.22	A
	ATOM	2040		GLU			52.618	17.459	29.991		44.90	A
	ATOM	2041	C	GLU			49.234	19.876	34.435		22.11	A
	ATOM	2042	o	GLU			49.147	19.161	35.437		20.27	A
20	ATOM	2042	N	GLU			49.276	21.204	34.506		18.40	A
20												
	ATOM	2044	CA	GLU			49.248	21.875	35.801		20.13	A
	MOTA	2045	CB	GLU			49.587	23.363	35.657		20.36	A
	MOTA	2046	CG	GLU			51.014	23.651	35.190		24.05	A
	MOTA	2047	CD	GLU		329	51.191	23.518	33.688		25.93	A
25	MOTA	2048		GLU			50.213	23.154	32.995		26.61	A
	MOTA	2049	OE2	GLU			52.311	23.781	33.198		27.19	A
	MOTA	2050	C	GLU	Α	329	47.890	21.718	36.480	1.00	19.36	A
	MOTA	2051	0	GLU	Α	329	47.775	21.879	37.694	1.00	18.74	A
	ATOM	2052	N	MET	Α	330	46.863	21.415	35.691	1.00	17.28	A
30	MOTA	2053	CA	MET	Α	330	45.520	21.220	36.229	1.00	16.38	A
	MOTA	2054	CB	MET	Α	330	44.474	21.833	35.294	1.00	17.65	A
	ATOM	2055	CG	MET			44.460	23.365	35.311		22.95	A
	ATOM	2056	SD	MET			44.186	24.026	36.979		26.78	A
	ATOM	2057	CE	MET			42.435	23.712	37.186		24.69	A
35	ATOM	2058	c	MET			45.257	19.730	36.422		14.30	A
	ATOM	2059	ō	MET			44.127	19.304	36.629		15.39	A
	ATOM	2060	N	GLU			46.327	18.949	36.346		15.60	A
	ATOM	2061	CA	GLU			46.289	17.501	36.531		17.08	A
	ATOM	2062	CB	GLU			45.607	17.155	37.862		17.00	A
40	ATOM	2062	CG	GLU			46.070	18.027	39.038		17.46	A
40			CD	GLU			47.591	18.179	39.145		20.16	
	ATOM	2064										A
	ATOM	2065		GLU			48.034	19.073	39.896		21.39	A
	MOTA	2066		GLU			48.345	17.420	38.500		18.87	A
	MOTA	2067	C	GLU			45.697	16.658	35.398		17.80	A
45	MOTA	2068	0	GLU			45.107	15.602	35.636		20.40	A
	MOTA	2069	N	GLY			45.844	17.133	34.167		16.23	A
	MOTA	2070	CA	GLY			45.420	16.353	33.015		14.10	A
	MOTA	2071	C	GLY	Α	332	43.982	16.154	32.596	1.00	13.54	A
	MOTA	2072	0	GLY	Α	332	43.063	16.864	33.017	1.00	11.96	A
50	ATOM	2073	N	TYR	Α	333	43.804	15.141	31.750	1.00	14.37	A
	MOTA	2074	CA	TYR	Α	333	42.510	14.806	31.182	1.00	13.56	A
	ATOM	2075	CB	TYR	Α	333	42.722	13.892	29.968	1.00	15.00	A
	ATOM	2076	CG	TYR			43.153	14.683	28.752		16.46	A
	ATOM	2077		TYR			42.206	15.172	27.849		15.29	A
55	ATOM	2078		TYR			42.573	16.002	26.794		13.42	A
22	ATOM	2079	CD2	TYR			44.490	15.039	28.561		14.91	A
	ATOM	2080	CE2	TYR			44.872	15.877	27.499		14.87	A
	ATOM	2081	CEZ	TYR			44.072	16.353	26.626		15.61	A
		2082	OH	TYR			44.244		25.599		17.29	A A
	ATOM	2082	UH	TIK	А	233	44.244	17.197	40.099	1.00	11.29	A

	ATOM	2083	C	TYR	Α	333	41.470	14.230	32.127	1.00	15.23	A
	ATOM	2084	0	TYR	А	333	40.278	14.323	31.846	1.00	16.63	A
	ATOM	2085	N	GLY			41.907	13.650	33.244		15.50	A
	MOTA	2086	CA	GLY			40.957	13.100	34.202		15.07	A
5	ATOM	2087	C	GLY			39.925	14.146	34.616		16.40	A
	MOTA	2088	0	GLY	Α	334	38.724	13.946	34.433	1.00	15.05	A
	ATOM	2089	N	PRO	Α	335	40.366	15.278	35.184	1.00	14.96	A
	ATOM	2090	CD	PRO	Δ	335	41.727	15.531	35.689	1 00	15.88	A
	ATOM	2091	CA			335	39.444	16.339	35.606		15.29	A
10	ATOM	2092	CB	PRO			40.383	17.397	36.178		13.19	A
10												
	MOTA	2093	CG			335	41.485	16.569	36.758		13.81	A
	ATOM	2094	C	PRO	Α	335	38.594	16.877	34.448	1.00	15.84	A
	ATOM	2095	0	PRO	Α	335	37.423	17.204	34.631	1.00	14.84	A
	ATOM	2096	N	LEU	Α	336	39.184	16.971	33.257	1.00	16.12	A
15	ATOM	2097	CA	LEU			38.450	17.465	32.094		15.52	A
	ATOM	2098	CB			336	39.396	17.653	30.898		14.39	A
	ATOM	2099	CG	LEU			38,770	17.991	29.538		15.46	A
	MOTA	2100		LEU			37.836	19.182	29.662		11.25	A
	MOTA	2101		LEU			39.884	18.285	28.528		14.11	A
20	MOTA	2102	С	LEU	Α	336	37.321	16.508	31.714	1.00	16.28	A
	ATOM	2103	0	LEU	Α	336	36.176	16.921	31.540	1.00	15.51	A
	ATOM	2104	N	LYS	Α	337	37.640	15.225	31.592	1.00	17.22	A
	ATOM	2105	CA	LYS			36.624	14.243	31.235		17.39	A
	ATOM	2106	CB	LYS			37.293	12.900	30.921		17.68	A
25	ATOM	2107	CG	LYS			38.170	12.994	29.676		22.31	A
23												
	ATOM	2108	CD	LYS			39.213	11.892	29.592		24.60	A
	MOTA	2109	CE	LYS			38.620	10.560	29.189		24.76	A
	MOTA	2110	NZ	LYS		337	39.710	9.560	28.997		25.05	A
	MOTA	2111	C	LYS	Α	337	35.577	14.096	32.342	1.00	17.33	A
30	ATOM	2112	0	LYS	Α	337	34.456	13.652	32.090	1.00	14.42	A
	ATOM	2113	N	ALA	Α	338	35.928	14.500	33.559	1.00	15.83	A
	ATOM	2114	CA	ALA			34.989	14.395	34.674		17.52	A
	ATOM	2115	CB	ALA			35.749	14.167	35.980		19.68	A
	ATOM	2116	C	ALA			34.095	15.621	34.804		18.83	A
2.5												
35	MOTA	2117	0	ALA			33.252	15.687	35.695		18.94	A
	ATOM	2118	N	HIS			34.262	16.596	33.918		19.42	A
	ATOM	2119	CA	HIS	Α	339	33.438	17.796	34.004	1.00	19.28	A
	MOTA	2120	CB	HIS	Α	339	33.865	18.819	32.949	1.00	19.20	A
	ATOM	2121	CG	HIS	Α	339	33.163	20.134	33.074	1.00	20.26	A
40	ATOM	2122	CD2	HIS	А	339	33.549	21.299	33.649	1.00	18.95	A
	ATOM	2123		HIS			31.880	20.340	32.612		19.10	A
	ATOM	2124		HIS			31.506	21.576	32.896		22.19	A
	ATOM	2125		HIS			32.500	22.179	33.525		21.98	A
	MOTA	2126	C	HIS			31.957	17.448	33.845		19.13	A
45	ATOM	2127	0	HIS			31.597	16.576	33.061		19.52	A
	MOTA	2128	N	PRO	Α	340	31.079	18.125	34.606	1.00	19.80	A
	MOTA	2129	CD	PRO	Α	340	31.424	19.119	35.640	1.00	19.08	A
	ATOM	2130	CA	PRO	Α	340	29.630	17.900	34.569	1.00	20.52	A
	ATOM	2131	CB	PRO			29.091	19.058	35.396		20.74	A
50	ATOM	2132	CG	PRO			30.146	19.207	36.454		19.20	A
50	ATOM	2133	C			340	29.000	17.834	33.176		21.42	A
	MOTA	2134	0	PRO			28.049	17.088	32.955		22.48	A
	MOTA	2135	N	PHE			29.528	18.606	32.237		21.33	A
	ATOM	2136	CA	PHE	Α	341	28.985	18.610	30.886	1.00	21.57	A
55	ATOM	2137	CB	PHE	Α	341	29.739	19.624	30.017	1.00	21.64	A
	ATOM	2138	CG	PHE	Α	341	29.207	19.740	28.613	1.00	23.18	A
	ATOM	2139		PHE			27.903	20.171	28.382		22.58	A
	ATOM	2140		PHE			30.013	19.431	27.522		21.95	A
	ATOM	2141		PHE			27.410	20.292	27.082		23.54	A
	TITOH	2141	CHI	2116	п	211	~1.410	20.252	27.002	1.00		А

	ATOM	2142	CE2	PHE .	A 34	41	29.533	19.548	26.220	1.00 21.83	A
	ATOM	2143	CZ	PHE .	3 3 4	41	28.228	19.980	25.998	1.00 23.23	A
	ATOM	2144	C	PHE .			29.055	17.226	30.237	1.00 21.84	A
	MOTA	2145	0	PHE .	4 34	41	28.232	16.896	29.389	1.00 20.37	A
5	ATOM	2146	N	PHE .	3 34	42	30.034	16.422	30.640	1.00 20.51	A
	MOTA	2147	CA	PHE .			30.221	15.085	30.077	1.00 23.01	A
	ATOM	2148	CB	PHE .	4 34	42	31.710	14.809	29.850	1.00 18.00	A
	ATOM	2149	CG	PHE .	A 34	42	32.398	15.812	28.971	1.00 17.05	A
	ATOM	2150	CD1	PHE .			32.010	15.987	27.652	1.00 17.78	A
10											
10	MOTA	2151		PHE .			33.487	16.534	29.450	1.00 15.72	A
	ATOM	2152	CE1	PHE .	A 34	42	32.702	16.867	26.811	1.00 18.08	A
	ATOM	2153	CE2	PHE .	A 34	42	34.184	17.414	28.617	1.00 17.45	A
	ATOM	2154	CZ	PHE .			33.790	17.578	27.298	1.00 16.56	A
	MOTA	2155	С	PHE .			29.679	13.972	30.976	1.00 24.95	A
15	ATOM	2156	0	PHE .	4 34	42	30.002	12.798	30.777	1.00 23.95	A
	ATOM	2157	N	GLU .	3 3 4	43	28.861	14.333	31.958	1.00 27.35	A
	ATOM	2158	CA	GLU .			28.325	13.349	32.897	1.00 30.28	A
	MOTA	2159	CB	GLU .			27.187	13.964	33.716	1.00 32.20	A
	ATOM	2160	CG	GLU .	A 34	43	26.581	12.991	34.714	1.00 39.71	A
20	MOTA	2161	CD	GLU .	3.4	43	25.628	13.661	35.688	1.00 44.72	A
	ATOM	2162		GLU .			24.661	14.314	35.234	1.00 47.55	A
	ATOM	2163	OE2	GLU .			25.847	13.526	36.911	1.00 46.89	A
	MOTA	2164	C	GLU .	A 34	43	27.852	12.017	32.305	1.00 28.98	A
	MOTA	2165	0	GLU .	3.4	4.3	28.225	10.952	32.800	1.00 31.73	A
25	ATOM	2166	N	SER .			27.037	12.067	31.258	1.00 26.09	A
23											
	MOTA	2167	CA	SER .			26.520	10.838	30.656	1.00 28.36	A
	MOTA	2168	CB	SER .	A 34	44	25.129	11.089	30.067	1.00 28.73	A
	ATOM	2169	OG	SER .	34	44	25.203	11.942	28.940	1.00 30.91	A
	ATOM	2170	C	SER .			27.407	10.214	29.577	1.00 27.66	A
30	MOTA	2171	0	SER .			26.987	9.281	28.900	1.00 28.66	A
	ATOM	2172	N	VAL .	4 34	45	28.627	10.715	29.419	1.00 26.75	A
	ATOM	2173	CA	VAL .	3 3 4	4.5	29.534	10.183	28.402	1.00 23.44	A
	ATOM	2174	CB	VAL .			30.565	11.256	27.950	1.00 23.10	A
	MOTA	2175		VAL .			31.589	10.631	26.995	1.00 22.24	A
35	MOTA	2176	CG2	VAL .	4 34	45	29.854	12.418	27.275	1.00 20.05	A
	ATOM	2177	C	VAL .	3 34	4.5	30.326	8.957	28.855	1.00 24.26	A
	ATOM	2178	ō	VAL .			30.876	8.930	29.960	1.00 22.83	A
	MOTA	2179	N	THR .			30.374	7.942	27.997	1.00 21.77	A
	MOTA	2180	CA	THR .	4 34	46	31.153	6.740	28.272	1.00 23.70	A
40	MOTA	2181	CB	THR .	34	46	30.391	5.455	27.857	1.00 26.53	A
	ATOM	2182		THR .			29.248	5.284	28.706	1.00 29.98	A
	MOTA	2183		THR .			31.289	4.231	27.990	1.00 24.28	A
	MOTA	2184	С	THR .	4 34	46	32.383	6.945	27.385	1.00 23.43	A
	ATOM	2185	0	THR .	A 34	46	32.306	6.827	26.160	1.00 24.50	A
45	ATOM	2186	N	TRP .			33.508	7.270	28.013	1.00 22.98	A
70											
	MOTA	2187	CA	TRP .			34.744	7.569	27.300	1.00 23.81	A
	MOTA	2188	CB	TRP .	A 34	47	35.683	8.352	28.219	1.00 22.54	A
	MOTA	2189	CG	TRP .	34	47	35.128	9.658	28.693	1.00 20.61	A
	ATOM	2190		TRP .			35.257	10.927	28.040	1.00 19.11	A
50											
50	MOTA	2191		TRP .			34.581	11.881	28.838	1.00 18.39	A
	MOTA	2192	CE3	TRP .	1 34	47	35.878	11.351	26.858	1.00 18.16	A
	ATOM	2193		TRP .			34.397	9.883	29.828	1.00 18.35	A
	ATOM	2194		TRP .			34.065	11.218	29.923	1.00 19.51	A
	MOTA	2195		TRP .			34.510	13.234	28.491	1.00 16.88	A
55	MOTA	2196	CZ3	TRP .	A 34	47	35.808	12.701	26.511	1.00 17.23	A
	ATOM	2197	CH2	TRP .	34	47	35.127	13.624	27.327	1.00 18.16	A
	ATOM	2198	C	TRP .			35.538	6.429	26.675	1.00 25.79	A
	ATOM	2199	0	TRP .			36.304	6.654	25.742	1.00 24.67	A
	MOTA	2200	N	ALA .	A 34	48	35.360	5.215	27.183	1.00 27.10	A

	ATOM	2201	CA	ALA	20	240	20	116	4.063	26.69	7 1 00	27.46	A
	MOTA	2202	CB	ALA				899	2.869	27.63		27.09	A
	ATOM	2203	C	ALA				895	3.620	25.25		27.18	A
	ATOM	2204	0	ALA	Α	348	36.	830	3.148	24.61	3 1.00	29.41	A
5	ATOM	2205	N	ASN	Α	349	34.	682	3.769	24.73	5 1.00	26.55	A
	ATOM	2206	CA	ASN				418	3.310	23.37		27.28	A
	ATOM	2207	CB	ASN				700	1.962	23.44		29.37	A
	MOTA	2208	CG	ASN				299	2.088	24.01		30.92	A
	MOTA	2209		ASN				045	2.942	24.85		30.17	A
10	MOTA	2210	ND2	ASN	Α	349	31.	386	1.237	23.55	3 1.00	33.52	A
	ATOM	2211	C	ASN	Α	349	33.	599	4.265	22.50	9 1.00	26.47	A
	ATOM	2212	0	ASN	Δ	349	32.	669	3.843	21.81	9 1.00	25.87	A
	ATOM	2213	N	LEU				947	5.543	22.51		24.45	A
	ATOM	2214	CA	LEU				203	6.510	21.72		23.14	A
15	MOTA	2215	CB	LEU				837	7.898	21.84		23.22	A
	MOTA	2216	CG	LEU	Α	350	33.	659	8.605	23.19	1 1.00	21.05	A
	MOTA	2217	CD1	LEU	Α	350	34.	646	9.756	23.29	3 1.00	19.36	A
	ATOM	2218	CD2	LEU	Α	350	32.	220	9.094	23.31	9 1.00	18.78	A
	ATOM	2219	C	LEU	Α	350	33.	082	6.152	20.24	1.00	22.60	A
20	ATOM	2220	ō	LEU				011	6.296	19.65		21.15	A
20	ATOM	2221	N	HIS				165	5.689	19.62		23.13	A
	MOTA	2222	CA	HIS				089	5.387	18.20		27.83	A
	MOTA	2223	CB	HIS				506	5.325	17.59		29.36	A
	ATOM	2224	CG	HIS	Α	351	36.	082	3.950	17.49	3 1.00	32.07	A
25	ATOM	2225	CD2	HIS	Α	351	36.	611	3.128	18.43	1 1.00	32.39	A
	ATOM	2226	ND1	HIS	Α	351	36.	197	3.285	16.29	1 1.00	33.02	A
	ATOM	2227	CE1	HIS	Α	351	36.	775	2.113	16.49	3 1.00	33.58	A
	ATOM	2228		HIS				036	1.992	17.78		31.76	A
	ATOM	2229	C	HIS				258	4.144	17.87		28.12	A
30	ATOM	2230	Ö	HIS				015	3.847	16.70		29.49	
30													A
	MOTA	2231	N	GLN				800	3.442	18.90		29.28	A
	MOTA	2232	CA	GLN				963	2.255	18.72		29.67	A
	MOTA	2233	CB	GLN	Α	352	32.	366	1.145	19.69	4 1.00	30.56	A
	ATOM	2234	CG	GLN	Α	352	33.	169	0.041	19.04	1 1.00	30.88	A
35	ATOM	2235	CD	GLN	Α	352	34.	493	-0.186	19.72	9 1.00	31.21	A
	ATOM	2236		GLN				541	-0.450	20.92		30.76	A
	ATOM	2237		GLN				578	-0.084	18.97		32.30	A
	ATOM	2238	C	GLN				504	2.638	18.96		30.42	A
	ATOM	2239	0	GLN				595	1.831	18.77		29.01	A
40	MOTA	2240	N	GLN				290	3.875	19.39		27.64	A
	MOTA	2241	CA	GLN				948	4.365	19.65		27.42	A
	ATOM	2242	CB	GLN	Α	353	28.	977	5.401	20.77	5 1.00	25.77	A
	ATOM	2243	CG	GLN	Α	353	29.	408	4.837	22.11	5 1.00	27.34	A
	ATOM	2244	CD	GLN	А	353	29.	638	5.914	23.15	6 1.00	27.19	A
45	ATOM	2245		GLN				875	6.872	23.25		28.29	A
75	ATOM	2246		GLN				687	5.753	23.95		28.79	A
	ATOM	2247	С	GLN				375	4.989	18.38		29.00	A
	MOTA	2248	0	GLN				118	5.455	17.51		29.14	A
	ATOM	2249	N	THR	А	354	27.	053	4.984	18.27	6 1.00	27.31	A
50	MOTA	2250	CA	THR	Α	354	26.	390	5.568	17.11	9 1.00	27.85	A
	ATOM	2251	CB	THR	Α	354	24.	991	4.941	16.90	4 1.00	30.69	A
	ATOM	2252	OG1	THR	А	354	25.	132	3.532	16.66	5 1.00	30.07	A
	ATOM	2253		THR				289	5.585	15.70		29.58	A
	ATOM	2254	C	THR				244	7.062	17.37		26.85	A
55													
23	MOTA	2255	0	THR				592	7.475	18.32		25.77	A
	ATOM	2256	N	PRO				867	7.898	16.53		27.22	A
	MOTA	2257	CD	PRO				792	7.588	15.43		25.89	A
	MOTA	2258	CA	PRO				763	9.346	16.73		27.23	A
	MOTA	2259	CB	PRO	Α	355	27.	625	9.915	15.60	9 1.00	24.91	A

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	MOTA	2260	CG			355	28.643	8.838	15.385		25.54	
	MOTA	2261	C	PRO	Α	355	25.322	9.837	16.641	1.00	28.07	
	ATOM	2262	0	PRO	Α	355	24.548	9.364	15.810	1.00	27.24	
	ATOM	2263	N	PRO	А	356	24.941	10.792	17.500	1.00	28.28	
5	ATOM	2264	CD			356	25.752	11.560	18.462		28.31	
,	ATOM	2265	CA			356	23.572	11.306	17.448		28.44	
	MOTA	2266	CB			356	23.539	12.301	18.604		28.11	
	MOTA	2267	CG			356	24.946	12.832	18.612		26.86	
	MOTA	2268	C			356	23.363	11.978	16.097		29.25	
10	MOTA	2269	0	PRO	Α	356	24.304	12.537	15.529	1.00	27.27	
	ATOM	2270	N	ALA	Α	357	22.143	11.910	15.575	1.00	30.45	
	MOTA	2271	CA	ALA	Α	357	21.848	12.521	14.287	1.00	32.81	
	MOTA	2272	CB	ALA			20.507	12.019	13.757		31.99	
	ATOM	2273	C	ALA			21.824	14.035	14.448		35.05	
15	ATOM	2274	ō	ALA			21.194	14.561	15.369		35.04	
13												
	ATOM	2275	N	LEU			22.516	14.730	13.552		37.81	
	MOTA	2276	CA	LEU			22.578	16.185	13.597		42.15	
	MOTA	2277	CB	LEU	Α	358	23.679	16.681	12.658	1.00	39.54	
	MOTA	2278	CG	LEU	Α	358	25.086	16.285	13.109	1.00	39.51	
20	ATOM	2279	CD1	LEU	Α	358	26.102	16.686	12.062	1.00	39.29	
	ATOM	2280	CD2	LEU	Α	358	25.395	16.953	14.445	1.00	40.01	
	ATOM	2281	С	LEU	А	358	21.241	16.837	13,242	1.00	45.91	
	ATOM	2282	ō	LEU			20.874	16.927	12.069		45.71	
	ATOM	2283	N	THR		359	20.530	17.290	14.275		50.06	
25	ATOM	2284	CA	THR			19.223	17.939	14.140		53.73	
23												
	ATOM	2285	CB	THR			19.353	19.428	13.726		54.04	
	MOTA	2286		THR			19.995	19.521	12.448		56.35	
	MOTA	2287	CG2	THR		359	20.158	20.204	14.763		54.32	
	ATOM	2288	C	THR	Α	359	18.309	17.236	13.139	1.00	54.47	
30	MOTA	2289	0	THR	Α	359	18.483	16.016	12.930	1.00	55.90	
	MOTA	2290	OXT	THR	Α	359	17.407	17.908	12.595	1.00	56.97	
	TER											
	ATOM	1	CB	PRO	B	71	99.838	54.646	-7.659	1.00	20.00	6
	ATOM	2	CG	PRO		71	99,216	55.105	-6.341		20.00	6
35	ATOM	3	C	PRO		71	98.903	54.776	-9.981		20.00	6
33	ATOM	4	ŏ	PRO		71	98.022		-10.109		20.00	8
	MOTA	5	N	PRO		71	97.782	55.851	-8.042		20.00	7
	MOTA	6	CD	PRO		71	97.728	55.323	-6.668		20.00	6
	MOTA	7	CA	PRO		71	99.087	55.515	-8.658		20.00	6
40	MOTA	8	N	PRO	В	72	99.732	55.097	-10.985	1.00	20.00	7
	MOTA	9	CD	PRO	В	72	100.794	56.121	-10.977	1.00	20.00	6
	ATOM	10	CA	PRO	В	72	99.645	54.451	-12.297	1.00	20.00	6
	ATOM	11	CB	PRO	В	72	100.885	54.973	-13.017	1.00	20.00	6
	ATOM	12	CG	PRO	В	72	101.026	56.352	-12.456	1.00	20.00	6
45	ATOM	13	C	PRO		72	99.627		-12.202		20.00	6
	ATOM	14	ō	PRO		72	100.246		-11.314		20.00	8
	ATOM	15	N	ALA		73	98.906		-13.122		20.00	7
	MOTA	16	CA	ALA		73	98.805		-13.167		20.00	6
	MOTA	17	CB	ALA		73	97.420		-12.710		20.00	6
50	MOTA	18	C	ALA		73	99.053		-14.604		20.00	6
	MOTA	19	0	ALA	В	73	99.027	51.215	-15.526	1.00	20.00	8
	ATOM	20	N	PRO	В	74	99.313	49.100	-14.818	1.00	20.00	7
	ATOM	21	CD	PRO	В	74	99.473	47.995	-13.857	1.00	20.00	6
	ATOM	22	CA	PRO		74	99.553		-16.189		20.00	6
55	ATOM	23	CB	PRO		74	99.700		-16.023		20.00	6
	ATOM	24	CG	PRO		74	100.292		-14.649		20.00	6
						74						
	MOTA	25	C	PRO			98.371		-17.079		20.00	6
	MOTA	26	0	PRO		74	97.279		-16.583		20.00	8
	MOTA	27	N	ALA	В	75	98.589	49.037	-18.389	1.00	20.00	7

	ATOM	28	CA	ALA	В	75	97.516	49.368 -19.321	1.00	20.00	6
	ATOM	29	CB	ALA	В	75	98.061	49.462 -20.745	1.00	20.00	6
	ATOM	30	C	ALA		75	96.446	48.285 -19.246		20.00	6
	ATOM	31	o	ALA		75	96.745	47.126 -18.961		20.00	8
5	ATOM	32	N	LYS		76	95.200	48.666 -19.494		20.00	7
3											
	MOTA	33	CA	LYS		76	94.098	47.716 -19.463		20.00	6
	MOTA	34	CB	LYS		76	92.793	48.431 -19.805		20.00	6
	ATOM	35	CG	LYS	В	76	91.546	47.792 -19.225	1.00	20.00	6
	MOTA	36	CD	LYS	В	76	91.511	47.932 -17.711	1.00	20.00	6
10	ATOM	37	CE	LYS	В	76	90.184	47.454 -17.152	1.00	20.00	6
	ATOM	38	NZ	LYS	В	76	90.108	47.606 -15.673	1.00	20.00	7
	ATOM	39	C	LYS		76	94.389	46.645 -20.513		20.00	6
	ATOM	40	o	LYS		76	94.736	46.968 -21.645		20.00	8
						77					7
15	ATOM	41	N	LYS			94.269	45.374 -20.145		20.00	
15	ATOM	42	CA	LYS		77	94.525	44.311 -21.107		20.00	6
	MOTA	43	CB	LYS		77	94.875	43.008 -20.384		20.00	6
	MOTA	44	CG	LYS	В	77	96.117	43.125 -19.506	1.00	20.00	6
	ATOM	45	CD	LYS	В	77	96.461	41.812 -18.842	1.00	20.00	6
	ATOM	46	CE	LYS	В	77	97.501	42.008 -17.745	1.00	20.00	6
20	ATOM	47	NZ	LYS	В	77	98.771	42.582 -18.255	1.00	20.00	7
	ATOM	48	С	LYS	В	77	93.311	44.111 -22.012	1.00	20.00	6
	ATOM	49	o	LYS		77	92.218	44.585 -21.704		20.00	8
	ATOM	50	N	ARG		78	93.514	43.418 -23.129		20.00	7
	ATOM	51	CA	ARG		78	92.442	43.158 -24.086		20.00	6
2.5											
25	ATOM	52	CB	ARG		78	92.465	44.224 -25.193		20.00	6
	MOTA	53	CG	ARG		78	93.787	44.344 -25.925		20.00	6
	MOTA	54	CD	ARG		78	93.833	45.612 -26.771		20.00	6
	ATOM	55	NE	ARG	В	78	95.052	45.702 -27.575	1.00	20.00	7
	ATOM	56	CZ	ARG	В	78	96.287	45.751 -27.078	1.00	20.00	6
30	ATOM	57	NH1	ARG	В	78	96.486	45.721 -25.764	1.00	20.00	7
	ATOM	58	NH2	ARG	В	78	97.330	45.828 -27.897	1.00	20.00	7
	ATOM	59	C	ARG		78	92.570	41.754 -24.678		20.00	6
	ATOM	60	Ö	ARG		78	93.625	41.126 -24.581		20.00	8
	ATOM	61	N	PRO		79	91.494	41.240 -25.303		20.00	7
2.5											
35	ATOM	62	CD	PRO		79	90.195	41.894 -25.543		20.00	6
	ATOM	63	CA	PRO		79	91.519	39.899 -25.896		20.00	6
	MOTA	64	CB	PRO		79	90.214	39.848 -26.691		20.00	6
	MOTA	65	CG	PRO	В	79	89.304	40.725 -25.889	1.00	20.00	6
	ATOM	66	C	PRO	В	79	92.737	39.614 -26.778	1.00	20.00	6
40	MOTA	67	0	PRO	В	79	93.311	38.523 -26.717	1.00	20.00	8
	ATOM	68	N	GLU	В	80	93.124	40.597 -27.589	1.00	20.00	7
	ATOM	69	CA	GLU	В	80	94.254	40.441 -28.503	1.00	20.00	6
	ATOM	70	CB	GLU		80	94.358	41.644 -29.446		20.00	6
	ATOM	71	CG	GLU		80	94.881	42.912 -28.800		20.00	6
45	ATOM	72	CD	GLU		80	95.009	44.057 -29.788		20.00	6
43											
	ATOM	73		GLU		80	93.968	44.513 -30.308		20.00	8
	ATOM	74		GLU		80	96.150	44.498 -30.047		20.00	8
	MOTA	75	C	GLU	В	80	95.591	40.235 -27.787		20.00	6
	MOTA	76	0	GLU	В	80	96.558	39.795 -28.405	1.00	20.00	8
50	MOTA	77	N	ASP	В	81	95.656	40.559 -26.497	1.00	20.00	7
	MOTA	78	CA	ASP	В	81	96.902	40.380 -25.749	1.00	20.00	6
	ATOM	79	CB	ASP		81	96.888	41.192 -24.446		20.00	6
	ATOM	80	CG	ASP		81	96.774	42.688 -24.682		20.00	6
	ATOM	81		ASP		81	97.436	43.193 -25.606		20.00	8
55	ATOM	82		ASP		81	96.033	43.362 -23.933		20.00	8
55	ATOM	83	C	ASP		81		38.914 -25.393		20.00	6
							97.111				
	MOTA	84	0	ASP		81	98.172	38.535 -24.890		20.00	8
	ATOM	85	N	PHE		82	96.103	38.093 -25.679		20.00	7
	ATOM	86	CA	PHE	В	82	96.140	36.677 -25.340	1.00	20.00	6

	MOTA	87	CB	PHE		82	95.056	36.369 -24.302	1.00 20.00	6
	MOTA	88	CG		В	82	95.157	37.187 -23.050	1.00 20.00	6
	MOTA	89		PHE	В	82	95.880	36.724 -21.959	1.00 20.00	6
	MOTA	90	CD2	PHE	В	82	94.525	38.423 -22.961	1.00 20.00	6
5	MOTA	91	CE1	PHE		82	95.976	37.479 -20.793	1.00 20.00	6
	MOTA	92	CE2	PHE	В	82	94.615	39.188 -21.800	1.00 20.00	6
	MOTA	93	CZ	PHE	В	82	95.343	38.712 -20.713	1.00 20.00	6
	MOTA	94	С		В	82	95.929	35.719 -26.496	1.00 20.00	6
	MOTA	95	0	PHE		82	95.342	36.061 -27.524	1.00 20.00	8
10	MOTA	96	N	LYS		83	96.406	34.500 -26.286	1.00 20.00	7
	MOTA	97	CA	LYS	В	83	96.242	33.411 -27.228	1.00 20.00	6
	MOTA	98	CB	LYS		83	97.594	32.777 -27.562	1.00 20.00	6
	MOTA	99	CG	LYS		83	97.503	31.531 -28.425	1.00 20.00	6
	MOTA	100	CD	LYS		83	98.888	31.074 -28.856	1.00 20.00	6
15	MOTA	101	CE	LYS		83	98.826	29.808 -29.699	1.00 20.00	6
	MOTA	102	NZ	LYS		83	98.287	28.654 -28.918	1.00 20.00	7
	MOTA	103	C	LYS		83	95.387	32.446 -26.416	1.00 20.00	6
	MOTA	104	0	LYS	В	83	95.884	31.776 -25.510	1.00 20.00	8
	MOTA	105	N		В	84	94.094	32.393 -26.710	1.00 20.00	7
20	MOTA	106	CA	PHE	В	84	93.217	31.511 -25.958	1.00 20.00	6
	ATOM	107	CB	PHE	В	84	91.758	31.928 -26.133	1.00 20.00	6
	MOTA	108	CG		В	84	91.426	33.228 -25.462	1.00 20.00	6
	MOTA	109	CD1	PHE	В	84	91.668	34.439 -26.099	1.00 20.00	6
	MOTA	110	CD2	PHE	В	84	90.907	33.243 -24.174	1.00 20.00	6
25	MOTA	111	CE1		В	84	91.400	35.644 -25.464	1.00 20.00	6
	ATOM	112	CE2	PHE	В	84	90.636	34.447 -23.528	1.00 20.00	6
	ATOM	113	CZ		В	84	90.884	35.646 -24.176	1.00 20.00	6
	MOTA	114	C	PHE	В	84	93.402	30.054 -26.335	1.00 20.00	6
	MOTA	115	0	PHE		84	93.734	29.734 -27.476	1.00 20.00	8
30	ATOM	116	N	GLY		85	93.196	29.178 -25.359	1.00 20.00	7
	ATOM	117	CA	GLY		85	93.349	27.758 -25.591	1.00 20.00	6
	ATOM	118	C	GLY		85	92.103	26.977 -25.221	1.00 20.00	6
	MOTA	119	0	GLY		85	90.982	27.393 -25.525	1.00 20.00	8
	MOTA	120	N	LYS	В	86	92.296	25.858 -24.534	1.00 20.00	7
35	ATOM	121	CA	LYS		86	91.182	25.005 -24.153	1.00 20.00	6
	MOTA	122	CB	LYS		86	91.695	23.640 -23.687	1.00 20.00	6
	MOTA	123	CG	LYS		86	92.421	23.667 -22.356	1.00 20.00	6
	MOTA	124	CD	LYS	В	86	92.855	22.272 -21.941	1.00 20.00	6
	MOTA	125	CE	LYS		86	93.685	22.319 -20.668	1.00 20.00	6
40	MOTA	126	NZ	LYS		86	94.209	20.975 -20.287	1.00 20.00	7
	MOTA	127	C	LYS		86	90.267	25.576 -23.077	1.00 20.00	6
	MOTA	128	0	LYS	В	86	90.668	26.410 -22.260	1.00 20.00	8
	ATOM	129	N		В	87	89.026	25.106 -23.102	1.00 20.00	7
	ATOM	130	CA	ILE	В	87	88.023	25.497 -22.131	1.00 20.00	6
45	ATOM	131	CB	ILE		87	86.604	25.159 -22.647	1.00 20.00	6
	MOTA	132		ILE	В	87	85.582	25.261 -21.503	1.00 20.00	6
	MOTA	133		ILE		87	86.260	26.085 -23.820	1.00 20.00	6
	MOTA	134		ILE		87	84.912	25.819 -24.463	1.00 20.00	6
	MOTA	135	С	ILE		87	88.312	24.687 -20.872	1.00 20.00	6
50	MOTA	136	0	ILE		87	88.396	23.461 -20.927	1.00 20.00	8
	MOTA	137	N	LEU		88	88.473	25.368 -19.742	1.00 20.00	7
	MOTA	138	CA	LEU		88	88.757	24.686 -18.486	1.00 20.00	6
	MOTA	139	CB	LEU		88	89.592	25.586 -17.575	1.00 20.00	6
	MOTA	140	CG	LEU		88	90.968	25.987 -18.112	1.00 20.00	6
55	MOTA	141		LEU		88	91.611	27.006 -17.186	1.00 20.00	6
	MOTA	142	CD2	LEU		88	91.836	24.756 -18.234	1.00 20.00	6
	MOTA	143	C	LEU		88	87.471	24.298 -17.776	1.00 20.00	6
	MOTA	144	0	LEU		88	87.434	23.334 -17.014	1.00 20.00	8
	ATOM	145	N	GLY	В	89	86.410	25.051 -18.024	1.00 20.00	7

	ATOM	146	CA	GLY	В	89	85.148	24.749 -17.382	1.00	20.00	6
	ATOM	147	C	GLY	В	89	84.038	25.599 -17.953	1.00	20.00	6
	ATOM	148	ō	GLY		89	84.296	26.657 -18.541		20.00	8
	ATOM	149	N	GLU		90	82.807	25.133 -17.781		20.00	7
5	ATOM	150	CA	GLU		90	81.629	25.832 -18.279		20.00	6
	ATOM	151	CB	GLU		90	81.041	25.070 -19.471		20.00	6
	ATOM	152	CG	GLU		90	81.929	25.084 -20.706		20.00	6
	ATOM	153	CD	GLU		90	81.434	24.157 -21.802		20.00	6
	ATOM	154		GLU		90	81.539	22.923 -21.639		20.00	8
10											
10	MOTA	155		GLU		90	80.935	24.662 -22.827		20.00	8
	MOTA	156	С	GLU		90	80.575	25.970 -17.188		20.00	6
	MOTA	157	0	GLU		90	80.208	24.994 -16.543		20.00	8
	MOTA	158	N	GLY		91	80.103	27.193 -16.979		20.00	7
	MOTA	159	CA	GLY		91	79.080	27.431 -15.979		20.00	6
15	MOTA	160	C	GLY		91	77.835	27.949 -16.673		20.00	6
	MOTA	161	0	GLY		91	77.804	28.046 -17.903		20.00	8
	MOTA	162	N	SER	В	92	76.808	28.291 -15.904	1.00	20.00	7
	MOTA	163	CA	SER	В	92	75.582	28.794 -16.508	1.00	20.00	6
	MOTA	164	CB	SER	В	92	74.428	28.719 -15.505	1.00	20.00	6
20	ATOM	165	OG	SER	В	92	74.786	29.335 -14.282	1.00	20.00	8
	ATOM	166	C	SER	В	92	75.726	30.219 -17.039	1.00	20.00	6
	ATOM	167	0	SER	В	92	75.078	30.585 -18.018	1.00	20.00	8
	ATOM	168	N	PHE	В	93	76.578	31.025 -16.411	1.00	20.00	7
	ATOM	169	CA	PHE	В	93	76.763	32.399 -16.870	1.00	20.00	6
25	ATOM	170	CB	PHE	В	93	76.276	33.384 -15.807	1.00	20.00	6
	ATOM	171	CG	PHE		93	74.832	33.220 -15.469		20.00	6
	ATOM	172			В	93	74.435	32.323 -14.483		20.00	6
	ATOM	173			В	93	73.859	33.914 -16.183		20.00	6
	ATOM	174		PHE		93	73.086	32.117 -14.210		20.00	6
30	ATOM	175	CE2	PHE		93	72.507	33.715 -15.919		20.00	6
50	ATOM	176	CZ	PHE		93	72.120	32.812 -14.930		20.00	6
	ATOM	177	c	PHE		93	78.197	32.736 -17.240		20.00	6
	ATOM	178	0	PHE		93	78.543	33.908 -17.397		20.00	8
	ATOM	179	N	SER		94	79.030	31.713 -17.394		20.00	7
25											
35	ATOM	180	CA	SER		94	80.421	31.948 -17.735		20.00	6
	ATOM	181	CB	SER		94	81.174	32.443 -16.503		20.00	6
	MOTA	182	OG	SER		94	81.237	31.410 -15.535		20.00	8
	MOTA	183	С	SER		94	81.123	30.707 -18.253		20.00	6
	MOTA	184	0	SER		94	80.666	29.584 -18.048		20.00	8
40	MOTA	185	N	THR		95	82.252	30.937 -18.913		20.00	7
	MOTA	186	CA	THR		95	83.088	29.879 -19.455		20.00	6
	MOTA	187	CB	THR		95	82.942	29.770 -20.985		20.00	6
	ATOM	188	OG1	THR	В	95	81.589	29.425 -21.309	1.00	20.00	8
	MOTA	189	CG2	THR	В	95	83.873	28.694 -21.536	1.00	20.00	6
45	MOTA	190	C	THR	В	95	84.524	30.264 -19.118	1.00	20.00	6
	ATOM	191	0	THR	В	95	84.957	31.388 -19.399	1.00	20.00	8
	ATOM	192	N	VAL	В	96	85.257	29.348 -18.498	1.00	20.00	7
	MOTA	193	CA	VAL	В	96	86.642	29.628 -18.141	1.00	20.00	6
	MOTA	194	CB	VAL	В	96	86.991	29.050 -16.761	1.00	20.00	6
50	ATOM	195	CG1	VAL	В	96	88.438	29.390 -16.407	1.00	20.00	6
	ATOM	196	CG2	VAL	В	96	86.041	29.627 -15.707	1.00	20.00	6
	ATOM	197	C	VAL		96	87.541	29.027 -19.210		20.00	6
	ATOM	198	ō	VAL		96	87.432	27.845 -19.540		20.00	8
	ATOM	199	N	VAL		97	88.416	29.858 -19.763		20.00	7
55	ATOM	200	CA	VAL		97	89.312	29.430 -20.824		20.00	6
	ATOM	201	CB	VAL		97	89.006	30.194 -22.130		20.00	6
	ATOM	202		VAL		97	89.828	29.624 -23.279		20.00	6
	ATOM	202		VAL		97	87.515	30.116 -22.444		20.00	6
	ATOM	203	C	VAL		97	90.771	29.664 -20.458		20.00	6
	MIUP	204	_	VPLL	D	21	50.11L	22.004 -20.438	1.00	40.00	0

	ATOM	205	0	VAL	В	97	91.122	30.698 -19.889	1.00 20.00	8
	ATOM	206	N	LEU	В	98	91.617	28.690 -20.770	1.00 20.00	7
	ATOM	207	CA	LEU	В	98	93.039	28.821 -20.499	1.00 20.00	6
	ATOM	208	CB	LEU	В	98	93.727	27.459 -20.618	1.00 20.00	6
5	ATOM	209	CG	LEU		98	95.240	27.421 -20.383	1.00 20.00	6
	ATOM	210		LEU		98	95.565	28.019 -19.021	1.00 20.00	6
	ATOM	211		LEU		98	95.739	25.987 -20.463	1.00 20.00	6
	ATOM	212	c	LEU		98	93.580	29.785 -21.552	1.00 20.00	6
	MOTA	213	ō	LEU		98	93.293	29.637 -22.738	1.00 20.00	8
10	ATOM	214	N	ALA		99	94.343	30.783 -21.121	1.00 20.00	7
	ATOM	215	CA	ALA		99	94.897	31.767 -22.043	1.00 20.00	6
	ATOM	216	CB	ALA		99	94.087	33.055 -21.980	1.00 20.00	6
	ATOM	217	C	ALA		99	96.353	32.067 -21.723	1.00 20.00	6
	ATOM	218	0	ALA		99	96.748	32.110 -20.554	1.00 20.00	8
15										
13	ATOM	219	N	ARG		100	97.152	32.270 -22.763	1.00 20.00	7
	ATOM	220	CA	ARG		100	98.554	32.596 -22.568	1.00 20.00	6
	MOTA	221	СВ	ARG			99.442	31.657 -23.393	1.00 20.00	6
	MOTA	222	CG	ARG		100	100.934	31.833 -23.131	1.00 20.00	6
	MOTA	223	CD	ARG		100	101.770	30.835 -23.923	1.00 20.00	6
20	MOTA	224	NE	ARG		100	101.600	29.452 -23.469	1.00 20.00	7
	MOTA	225	CZ	ARG			102.059	28.970 -22.314	1.00 20.00	6
	MOTA	226		ARG			102.722	29.752 -21.473	1.00 20.00	7
	MOTA	227		ARG			101.864	27.694 -22.003	1.00 20.00	7
	MOTA	228	C	ARG			98.756	34.045 -23.004	1.00 20.00	6
25	MOTA	229	0	ARG			98.454	34.408 -24.146	1.00 20.00	8
	MOTA	230	N	GLU			99.228	34.883 -22.087	1.00 20.00	7
	MOTA	231	CA	GLU			99.470	36.286 -22.408	1.00 20.00	6
	ATOM	232	CB	GLU			99.709	37.091 -21.123	1.00 20.00	6
	MOTA	233	CG	GLU		101	99.986	38.571 -21.363	1.00 20.00	6
30	ATOM	234	CD	GLU		101	100.164	39.347 -20.075	1.00 20.00	6
	MOTA	235		GLU			100.717	38.780 -19.114	1.00 20.00	8
	ATOM	236	OE2	GLU	В	101	99.765	40.531 -20.025	1.00 20.00	8
	MOTA	237	C	GLU	В	101	100.703	36.338 -23.317	1.00 20.00	6
	MOTA	238	0	GLU	В	101	101.773	35.865 -22.944	1.00 20.00	8
35	ATOM	239	N	LEU	В	102	100.546	36.909 -24.507	1.00 20.00	7
	ATOM	240	CA	LEU	В	102	101.632	36.982 -25.482	1.00 20.00	6
	ATOM	241	CB	LEU	В	102	101.145	37.683 -26.753	1.00 20.00	6
	ATOM	242	CG	LEU	В	102	100.013	36.985 -27.517	1.00 20.00	6
	ATOM	243	CD1	LEU	В	102	99.500	37.897 -28.623	1.00 20.00	6
40	ATOM	244	CD2	LEU	В	102	100.517	35.670 -28.089	1.00 20.00	6
	ATOM	245	C	LEU	В	102	102.906	37.663 -25.000	1.00 20.00	6
	ATOM	246	0	LEU	В	102	104.000	37.137 -25.180	1.00 20.00	8
	ATOM	247	N	ALA	В	103	102.760	38.828 -24.382	1.00 20.00	7
	ATOM	248	CA	ALA	В	103	103.909	39.587 -23.910	1.00 20.00	6
45	ATOM	249	CB	ALA	В	103	103.464	41.002 -23.546	1.00 20.00	6
	ATOM	250	C	ALA	В	103	104.697	38.983 -22.747	1.00 20.00	6
	ATOM	251	0	ALA	В	103	105.832	39.389 -22.503	1.00 20.00	8
	ATOM	252	N	THR			104.122	38.007 -22.050	1.00 20.00	7
	ATOM	253	CA	THR			104.790	37.418 -20.893	1.00 20.00	6
50	ATOM	254	СВ	THR			104.059	37.799 -19.592	1.00 20.00	6
	ATOM	255	OG1	THR			102.712	37.303 -19.648	1.00 20.00	8
	ATOM	256	CG2	THR			104.033	39.313 -19.404	1.00 20.00	6
	ATOM	257	c	THR		104	104.880	35.902 -20.901	1.00 20.00	6
	ATOM	258	ō	THR			105.677	35.323 -20.160	1.00 20.00	8
55	ATOM	259	N	SER			104.042	35.274 -21.722	1.00 20.00	7
	ATOM	260	CA			105	103.950	33.818 -21.842	1.00 20.00	6
	ATOM	261	CB	SER		105	105.344	33.213 -22.048	1.00 20.00	6
	ATOM	262	OG	SER			105.264	31.819 -22.287	1.00 20.00	8
	ATOM	263	C			105	103.204	33.243 -20.576	1.00 20.00	6

	ATOM	264	0	SER	_	105	103.286	32.029	00 262	1.00 20.00	8
	MOTA	265	N	ARG			102.771	34.124		1.00 20.00	7
	MOTA	266	CA	ARG			102.089	33.709		1.00 20.00	6
	MOTA	267	CB	ARG	В	106	101.833	34.914	-17.598	1.00 20.00	6
5	ATOM	268	CG	ARG	В	106	103.022	35.361	-16.781	1.00 20.00	6
	MOTA	269	CD	ARG	В	106	102.724	36.653	-16.045	1.00 20.00	6
	ATOM	270	NE	ARG			103.756	36.940		1.00 20.00	7
	ATOM	271	CZ	ARG			103.964	38.132		1.00 20.00	6
	ATOM	272		ARG			103.210	39.167		1.00 20.00	7
10		273		ARG			104.918	38.279		1.00 20.00	7
10	ATOM										
	MOTA	274	C	ARG			100.743	33.082		1.00 20.00	6
	ATOM	275	0	ARG			100.069	33.534		1.00 20.00	8
	MOTA	276	N	GLU	В	107	100.354	32.049	-18.115	1.00 20.00	7
	ATOM	277	CA	GLU	В	107	99.072	31.390	-18.336	1.00 20.00	6
15	ATOM	278	CB	GLU	В	107	99.193	29.870	-18.212	1.00 20.00	6
	ATOM	279	CG	GLU			100.180	29.207		1.00 20.00	6
	ATOM	280	CD	GLU			100.124	27.696		1.00 20.00	6
	ATOM	281		GLU			99.373	27.068		1.00 20.00	8
20	ATOM	282		GLU			100.813	27.144		1.00 20.00	8
20	MOTA	283	Ç	GLU			98.070	31.848		1.00 20.00	6
	ATOM	284	0	GLU			98.368	31.833		1.00 20.00	8
	MOTA	285	N	TYR			96.885	32.243	-17.727	1.00 20.00	7
	ATOM	286	CA	TYR	В	108	95.829	32.667	-16.817	1.00 20.00	6
	ATOM	287	CB	TYR	В	108	95.525	34.156	-16.979	1.00 20.00	6
25	ATOM	288	CG	TYR	В	108	96.603	35.089		1.00 20.00	6
	ATOM	289	CD1	TYR			96.744	35.369		1.00 20.00	6
	ATOM	290		TYR			97.727	36.260		1.00 20.00	6
	ATOM	291		TYR			97.467	35.712		1.00 20.00	6
	MOTA	292	CE2	TYR			98.442	36.597		1.00 20.00	6
30	ATOM	293	CZ	TYR			98.569	36.869		1.00 20.00	6
	ATOM	294	OH	TYR			99.529	37.756		1.00 20.00	8
	MOTA	295	С	TYR	В	108	94.566	31.899	-17.167	1.00 20.00	6
	MOTA	296	0	TYR	В	108	94.389	31.463	-18.306	1.00 20.00	8
	ATOM	297	N	ALA	В	109	93.697	31.723	-16.181	1.00 20.00	7
35	ATOM	298	CA	ALA	В	109	92.421	31.073	-16.414	1.00 20.00	6
	ATOM	299	CB	ALA			92.024	30.225		1.00 20.00	6
	ATOM	300	c	ALA			91.513	32.288		1.00 20.00	6
	ATOM	301	ō	ALA			91.278	33.003		1.00 20.00	8
40	ATOM	302	N	ILE			91.042	32.557		1.00 20.00	7
40	MOTA	303	CA	ILE			90.186	33.711		1.00 20.00	6
	MOTA	304	CB	ILE			90.574	34.462		1.00 20.00	6
	ATOM	305		ILE			89.628	35.630		1.00 20.00	6
	MOTA	306		ILE			92.023	34.962	-19.159	1.00 20.00	6
	ATOM	307	CD1	ILE	В	110	92.487	35.847	-20.312	1.00 20.00	6
45	ATOM	308	C	ILE	В	110	88.715	33.318	-18.004	1.00 20.00	6
	ATOM	309	0	ILE			88.285	32.527	-18.851	1.00 20.00	8
	ATOM	310	N	LYS			87.956	33.852		1.00 20.00	7
	ATOM	311	CA	LYS			86.527	33.581		1.00 20.00	6
	ATOM	312	CB	LYS			86.022	33.721		1.00 20.00	6
50											
50	MOTA	313	CG	LYS			84.509	33.598		1.00 20.00	6
	MOTA	314	CD	LYS			84.025	33.590		1.00 20.00	6
	ATOM	315	CE	LYS			84.318	32.262		1.00 20.00	6
	MOTA	316	NZ	LYS			83.784	32.217		1.00 20.00	7
	MOTA	317	C	LYS	В	111	85.844	34.601	-17.869	1.00 20.00	6
55	MOTA	318	0	LYS	В	111	86.017	35.807	-17.688	1.00 20.00	8
	ATOM	319	N	ILE			85.078	34.111		1.00 20.00	7
	ATOM	320	CA	ILE			84.383	34.976		1.00 20.00	6
	ATOM	321	CB	ILE			84.695	34.548		1.00 20.00	6
		322		ILE							
	ATOM	322	CGZ	TPR	ದ	112	84.042	35.505	-22.216	1.00 20.00	6

	MOTA	323	CG1	ILE	В	112	86.216	34.518 -21.440	1.00 2		6
	ATOM	324	CD1	ILE	В	112	86.657	33.949 -22.779	1.00 2	20.00	6
	ATOM	325	C	ILE	В	112	82.878	34.916 -19.538	1.00 2	20.00	6
	ATOM	326	ō	ILE			82.288	33.839 -19.510	1.00		8
-											
5	MOTA	327	N	LEU			82.269	36.083 -19.347	1.00 2		7
	MOTA	328	CA	LEU	В	113	80.835	36.172 -19.089	1.00 2	20.00	6
	ATOM	329	CB	LEU	В	113	80.585	36.696 -17.669	1.00 2	20.00	6
	ATOM	330	CG	LEU			81.350	36.038 -16.521	1.00 2		6
	ATOM	331		LEU			82.743	36.638 -16.428	1.00		6
10											
10	MOTA	332		LEU			80.609	36.258 -15.215	1.00		6
	MOTA	333	C	LEU	В	113	80.172	37.110 -20.090	1.00 2	20.00	6
	ATOM	334	0	LEU	В	113	80.634	38.232 -20.299	1.00 2	20.00	8
	ATOM	335	N	GLU	B	114	79.088	36.653 -20.709	1.00 2	20 00	7
	ATOM	336	CA	GLU			78.377	37.472 -21.681	1.00		6
15	MOTA	337	CB	GLU			77.514	36.586 -22.581	1.00 2		6
	ATOM	338	CG	GLU	В	114	76.670	37.366 -23.571	1.00 2	20.00	6
	ATOM	339	CD	GLU	В	114	75.749	36.473 -24.372	1.00 2	20.00	6
	ATOM	340	OE1	GLU	В	114	75.083	35.613 -23.760	1.00 2	20.00	8
	ATOM	341	OE2	GLU			75.684	36.638 -25.611	1.00		8
20											
20	MOTA	342	C	GLU			77.509	38.491 -20.942	1.00 2		6
	MOTA	343	0	GLU			76.673	38.122 -20.113	1.00 2		8
	ATOM	344	N	LYS	В	115	77.709	39.771 -21.235	1.00 2	20.00	7
	ATOM	345	CA	LYS	В	115	76.945	40.808 -20.553	1.00 2	20.00	6
	ATOM	346	CB	LYS		115	77.433	42.202 -20.978	1.00		6
25		347	CG	LYS				42.675 -20.183			6
23	MOTA						78.653		1.00		
	MOTA	348	CD	LYS			79.174	44.045 -20.618	1.00 2		6
	MOTA	349	CE	LYS	В	115	79.832	43.994 -21.992	1.00 2	20.00	6
	ATOM	350	NZ	LYS	В	115	80.536	45.273 -22.323	1.00 2	20.00	7
	ATOM	351	С	LYS			75.435	40.693 -20.743	1.00 2		6
30	ATOM	352	ō	LYS			74.676	40.787 -19.778	1.00		8
30											
	MOTA	353	N	ARG		116	74.997	40.471 -21.977	1.00 2		7
	MOTA	354	CA	ARG	В	116	73.570	40.363 -22.255	1.00 2	20.00	6
	ATOM	355	CB	ARG	В	116	73.346	40.066 -23.743	1.00 2	20.00	6
	ATOM	356	CG	ARG	В	116	71.893	39.821 -24.142	1.00 2	20.00	6
35	ATOM	357	CD	ARG		116	70.931	40.791 -23.465	1.00		6
55											
	MOTA	358	NE	ARG			71.401	42.172 -23.493	1.00		7
	MOTA	359	CZ	ARG			70.780	43.177 -22.884	1.00 2		6
	MOTA	360	NH1	ARG	В	116	69.663	42.949 -22.207	1.00 2	20.00	7
	ATOM	361	NH2	ARG	В	116	71.278	44.405 -22.942	1.00 2	20.00	7
40	ATOM	362	С	ARG	В	116	72.888	39.298 -21.394	1.00 2	20.00	6
	ATOM	363	ō	ARG			71.862	39.567 -20.764	1.00		8
	ATOM	364	N	HIS			73.463	38.101 -21.347	1.00		7
	MOTA	365	CA	HIS			72.885	37.020 -20.556	1.00 2		6
	MOTA	366	CB	HIS	В	117	73.704	35.738 -20.723	1.00 2	20.00	6
45	ATOM	367	CG	HIS	В	117	73.053	34.525 -20.133	1.00 2	20.00	6
	ATOM	368	CD2	HIS	В	117	71.762	34.274 -19.810	1.00 2	20.00	6
	ATOM	369		HIS		117	73.752	33.376 -19.836	1.00		7
	MOTA	370		HIS			72.921	32.467 -19.355	1.00 2		6
	MOTA	371		HIS			71.707	32.987 -19.330	1.00 2		7
50	ATOM	372	С	HIS	В	117	72.816	37.386 -19.077	1.00 2	20.00	6
	ATOM	373	0	HIS	В	117	71.823	37.113 -18.409	1.00 2	20.00	8
	ATOM	374	N	ILE			73.882	37.992 -18.564	1.00		7
	MOTA	375	CA	ILE			73.927	38.391 -17.160	1.00 2		6
	MOTA	376	CB	ILE		118	75.269	39.073 -16.827	1.00		6
55	MOTA	377	CG2	ILE	В	118	75.180	39.787 -15.486	1.00 2	20.00	6
	ATOM	378	CG1	ILE	В	118	76.392	38.029 -16.834	1.00 2	20.00	6
	ATOM	379		ILE		118	77.784	38.625 -16.709	1.00		6
	MOTA	380	С	ILE			72.788	39.353 -16.833	1.00 2		6
	MOTA	381	0	ILE	В	118	72.101	39.196 -15.827	1.00 2	20.00	8

	ATOM	382	N	ILE	В	119	72.596	40.349	-17.690	1.00	20.00	7
	ATOM	383	CA	ILE	В	119	71.538	41.333	-17.494	1.00	20.00	6
	ATOM	384	CB	ILE	В	119	71.646	42.473	-18.539	1.00	20.00	6
	ATOM	385	CG2	ILE			70.396	43.357	-18.492	1.00	20.00	6
5	ATOM	386		ILE			72.919		-18.270	1.00		6
	ATOM	387					73.212		-19.314	1.00		6
	ATOM	388	C	ILE			70.154		-17.580	1.00		6
	ATOM	389	ō	ILE			69.289		-16.747	1.00		8
	ATOM	390	N	LYS			69.950		-18.579	1.00		7
10	ATOM	391	CA	LYS			68.659		-18.754		20.00	6
10	ATOM	392	CB	LYS			68.697		-19.935		20.00	6
		393	CG	LYS			68.942		-19.935		20.00	6
	ATOM	394	CD	LYS			68.926		-21.204		20.00	6
	ATOM											
	ATOM	395	CE	LYS			69.934		-22.093		20.00	6
15	ATOM	396	NZ	LYS			69.950		-23.127		20.00	7
	ATOM	397	C	LYS			68.229		-17.513	1.00		6
	MOTA	398	0	LYS			67.077		-17.092	1.00		8
	MOTA	399	N	GLU			69.154		-16.930	1.00		7
	MOTA	400	CA	GLU			68.851		-15.747		20.00	6
20	ATOM	401	CB	GLU			69.678		-15.758		20.00	6
	ATOM	402	CG	GLU			69.485		-16.995	1.00		6
	ATOM	403	CD	GLU			68.029		-17.248		20.00	6
	MOTA	404		GLU			67.339	33.904	-16.295	1.00	20.00	8
	MOTA	405	OE2	GLU	В	121	67.574		-18.404	1.00	20.00	8
25	ATOM	406	C	GLU	В	121	69.071	37.573	-14.424	1.00	20.00	6
	ATOM	407	0	GLU	В	121	69.117	36.946	-13.362	1.00	20.00	8
	ATOM	408	N	ASN	В	122	69.208	38.895	-14.485	1.00	20.00	7
	ATOM	409	CA	ASN	В	122	69.411	39.699	-13.281	1.00	20.00	6
	ATOM	410	CB	ASN	В	122	68.132	39.715	-12.439	1.00	20.00	6
30	ATOM	411	CG	ASN	В	122	66.952	40.314	-13.177	1.00	20.00	6
	ATOM	412	OD1	ASN	В	122	66.428	39.725	-14.121	1.00	20.00	8
	ATOM	413		ASN			66.530		-12.748	1.00		7
	ATOM	414	С	ASN			70.563		-12.419		20.00	6
	ATOM	415	0	ASN			70.408		-11.212	1.00		8
35	ATOM	416	N	LYS			71.716		-13.033	1.00		7
	ATOM	417	CA	LYS			72.870		-12.301	1.00		6
	ATOM	418	СВ	LYS			73.500		-13.065		20.00	6
	ATOM	419	CG	LYS			72.568		-13.276		20.00	6
	ATOM	420	CD	LYS			72.065		-11.948	1.00		6
40	ATOM	421	CE	LYS			71.032		-12.159	1.00		6
	ATOM	422	NZ	LYS			70.421		-10.871		20.00	7
	ATOM	423	c	LYS			73.931		-12.054	1.00		6
	ATOM	424	Ö	LYS			75.035		-11.611	1.00		8
	ATOM	425	N	VAL			73.607		-12.340	1.00		7
45	ATOM	426	CA	VAL			74.575		-12.145		20.00	6
75	ATOM	427	CB	VAL			73.997		-12.547		20.00	6
	ATOM	428		VAL			75.035		-12.347	1.00		6
	ATOM	429		VAL			73.608		-14.022	1.00		6
50	ATOM	430	C	VAL			75.091		-10.712		20.00	6
30	ATOM	431	0	VAL			76.278		-10.490	1.00		8
	ATOM	432	N	PRO			74.207	41.695	-9.716	1.00		7
	ATOM	433	CD	PRO			72.735	41.613	-9.757	1.00		6
	MOTA	434	CA	PRO			74.688	41.747	-8.331	1.00		6
	ATOM	435	CB	PRO			73.411	41.558	-7.512		20.00	6
55	MOTA	436	CG	PRO			72.346	42.152	-8.396	1.00		6
	MOTA	437	C	PRO			75.715	40.643	-8.051	1.00		6
	MOTA	438	0	PRO			76.683	40.851	-7.325	1.00		8
	MOTA	439	N	TYR			75.493	39.475	-8.640		20.00	7
	MOTA	440	CA	TYR	В	126	76.380	38.334	-8.440	1.00	20.00	6

	ATOM	441	CB	TYR	В	126	75.699	37.059	-8.942	1.00	20.00	6
	ATOM	442	CG			126	74.479	36.687	-8.127		20.00	6
	ATOM	443		TYR			74.611	36.068	-6.884		20.00	6
	ATOM	444		TYR		126	73.491	35.748	-6.112		20.00	6
5	ATOM	445	CD2	TYR		126	73.193	36.981	-8.583		20.00	6
	ATOM	446	CE2	TYR		126	72.063	36.667	-7.817		20.00	6
	ATOM	447	CZ	TYR		126	72.223	36.052	-6.584		20.00	6
	ATOM	448	OH	TYR			71.118	35.743	-5.823		20.00	8
	ATOM	449	C	TYR			77.738	38.511	-9.113		20.00	6
10												
10	ATOM	450	0	TYR			78.777	38.273	-8.492		20.00	8
	MOTA	451	N	VAL		127	77.738		-10.374		20.00	7
	ATOM	452	CA	VAL		127	78.994		-11.085		20.00	6
	MOTA	453	CB	VAL		127	78.756		-12.567		20.00	6
	MOTA	454		VAL		127	80.096		-13.275		20.00	6
15	MOTA	455	CG2	VAL		127	77.949		-13.234		20.00	6
	MOTA	456	C	VAL		127	79.798		-10.427		20.00	6
	MOTA	457	0	VAL		127	81.016		-10.292		20.00	8
	ATOM	458	N	THR		128	79.105		-10.006		20.00	7
	ATOM	459	CA	THR		128	79.746	42.424	-9.345		20.00	6
20	MOTA	460	CB	THR	В	128	78.721	43.548	-9.070	1.00	20.00	6
	MOTA	461	OG1	THR	В	128	78.194	44.025	-10.316	1.00	20.00	8
	MOTA	462	CG2	THR	В	128	79.371	44.703	-8.330	1.00	20.00	6
	ATOM	463	C	THR	В	128	80.372	41.979	-8.019	1.00	20.00	6
	ATOM	464	0	THR	В	128	81.500	42.355	-7.696	1.00	20.00	8
25	ATOM	465	N	ARG	В	129	79.637	41.172	-7.256	1.00	20.00	7
	ATOM	466	CA	ARG	В	129	80.126	40.678	-5.971	1.00	20.00	6
	ATOM	467	CB	ARG	В	129	79.035	39.888	-5.254	1.00	20.00	6
	ATOM	468	CG	ARG	В	129	79.428	39.438	-3.852	1.00	20.00	6
	ATOM	469	CD	ARG	В	129	78.351	38.554	-3.278	1.00	20.00	6
30	ATOM	470	NE	ARG	В	129	77.048	39.209	-3.315	1.00	20.00	7
	ATOM	471	CZ	ARG	В	129	75.894	38.569	-3.484	1.00	20.00	6
	ATOM	472	NH1	ARG	В	129	75.878	37.250	-3.636	1.00	20.00	7
	ATOM	473	NH2	ARG	В	129	74.756	39.248	-3.501	1.00	20.00	7
	ATOM	474	С	ARG	В	129	81.354	39.788	-6.146	1.00	20.00	6
35	ATOM	475	0	ARG	В	129	82.315	39.885	-5.379		20.00	8
	ATOM	476	N	GLU			81.316	38.917	-7.151		20.00	7
	ATOM	477	CA	GLU			82.439	38.029	-7.421		20.00	6
	ATOM	478	CB	GLU		130	82.191	37.211	-8.692		20.00	6
	ATOM	479	CG	GLU		130	83.408	36.427	-9.167		20.00	6
40	ATOM	480	CD	GLU		130	83.060		-10.168		20.00	6
	ATOM	481		GLU		130	82.227		-11.061		20.00	8
	ATOM	482		GLU		130	83.626		-10.068		20.00	8
	ATOM	483	C	GLU		130	83.708	38.853	-7.580		20.00	6
	ATOM	484	ō	GLU		130	84.723	38.575	-6.940		20.00	8
45	ATOM	485	N	ARG		131	83.641	39.874	-8.428		20.00	7
	ATOM	486	CA	ARG		131	84.788	40.742	-8.673		20.00	6
	ATOM	487	CB	ARG			84.459	41.759	-9.777		20.00	6
	ATOM	488	CG	ARG		131	85.580		-10.035		20.00	6
	ATOM	489	CD	ARG			85.262		-11.167		20.00	6
50	ATOM	490	NE	ARG		131	86.351		-11.355		20.00	7
50	ATOM	491	CZ	ARG			86.416		-12.343		20.00	6
	ATOM	491		ARG			85.450		-13.250		20.00	7
	ATOM	492		ARG		131	87.450		-12.426		20.00	7
		493	NH2 C								20.00	
55	ATOM		0	ARG		131	85.228	41.485	-7.409			6
23	ATOM	495		ARG			86.413	41.500	-7.071		20.00	
	MOTA	496	N	ASP			84.277	42.103	-6.715		20.00	7
	ATOM	497	CA	ASP		132	84.594	42.848	-5.505		20.00	6
	MOTA	498	CB	ASP			83.350	43.575	-4.987		20.00	6
	MOTA	499	CG	ASP	В	132	82.865	44.658	-5.943	1.00	20.00	6

	ATOM	500		ASP			83.612	45.010	-6.886		20.00	8
	ATOM	501		ASP			81.739	45.167	-5.747		20.00	8
	ATOM	502	C	ASP			85.192	41.969	-4.401		20.00	6
	ATOM	503	0	ASP		132	86.191	42.337	-3.783		20.00	8
5	MOTA	504	N	VAL		133	84.596	40.809	-4.150		20.00	7
	MOTA	505	CA	VAL		133	85.131	39.933	-3.116		20.00	6
	MOTA	506	CB	VAL		133	84.226	38.698	-2.885		20.00	6
	MOTA	507		VAL		133	84.920	37.713	-1.957		20.00	6
	MOTA	508	CG2	VAL		133	82.893	39.135	-2.271		20.00	6
10	ATOM	509	C	VAL		133	86.540	39.470	-3.477		20.00	6
	MOTA	510	0	VAL		133	87.460	39.602	-2.675		20.00	8
	ATOM	511	N	MET		134	86.721	38.950	-4.688		20.00	7
	MOTA	512	CA			134	88.040	38.474	-5.083		20.00	6
	MOTA	513	CB	MET		134	88.004	37.879	-6.492		20.00	6
15	MOTA	514	CG			134	87.183	36.603	-6.573		20.00	6
	ATOM	515	SD	MET		134	87.477	35.650	-8.077		20.00	16
	MOTA	516	CE	MET			88.730	34.515	-7.475		20.00	6
	MOTA	517	С	MET		134	89.115	39.552	-4.994		20.00	6
	MOTA	518	0	MET		134	90.253	39.264	-4.626		20.00	8
20	MOTA	519	N	SER			88.758	40.790	-5.319		20.00	7
	ATOM	520	CA	SER			89.708	41.899	-5.260		20.00	6
	MOTA	521	CB	SER		135	89.084	43.175	-5.836		20.00	6
	MOTA	522	OG	SER			88.742	43.009	-7.202		20.00	8
	MOTA	523	C	SER			90.165	42.184	-3.830		20.00	6
25	MOTA	524	0	SER			91.228	42.762	-3.614		20.00	8
	MOTA	525	N	ARG		136	89.354	41.782	-2.857		20.00	7
	MOTA	526	CA	ARG		136	89.672	42.013	-1.450		20.00	6
	MOTA	527	CB	ARG			88.384	42.156	-0.637		20.00	6
	MOTA	528	CG	ARG		136	87.509	43.336	-1.018		20.00	6
30	MOTA	529	CD	ARG		136	86.215	43.306	-0.211		20.00	6
	MOTA	530	NE	ARG		136	86.491	43.117	1.209		20.00	7
	MOTA	531	CZ	ARG		136	85.565	42.888	2.132		20.00	6
	MOTA	532		ARG			84.285	42.821	1.786		20.00	7
	MOTA	533		ARG			85.920	42.715	3.401		20.00	7
35	ATOM	534	C	ARG			90.506	40.891	-0.839		20.00	6
	MOTA	535	0	ARG			91.091	41.054	0.231		20.00	8
	MOTA	536	N	LEU		137	90.556	39.752	-1.515		20.00	7
	MOTA	537	CA	LEU		137	91.300	38.609	-1.005		20.00	6
	MOTA	538	CB	LEU			90.665	37.307	-1.504		20.00	6
40	MOTA	539	CG	LEU			89.172	37.099	-1.213		20.00	6
	MOTA	540		LEU			88.748	35.728	-1.734		20.00	6
	ATOM	541		LEU			88.897	37.205	0.280		20.00	6
	ATOM	542	С	LEU			92.771	38.648	-1.402		20.00	6
	ATOM	543	0	LEU			93.103	38.871	-2.566		20.00	8
45	MOTA	544	N	ASP			93.645	38.436	-0.424		20.00	7
	MOTA	545	CA	ASP		138	95.086	38.422	-0.656		20.00	6
	MOTA	546	CB	ASP			95.696	39.797	-0.352		20.00	6
	ATOM	547	CG	ASP		138	97.179	39.854	-0.674		20.00	6
	ATOM	548		ASP			97.601	39.173	-1.634		20.00	8
50	MOTA	549		ASP		138	97.920	40.581	0.022		20.00	8
	MOTA	550	C	ASP		138	95.678	37.369	0.263		20.00	6
	MOTA	551	0	ASP		138	96.353	37.685	1.243		20.00	8
	MOTA	552	N	HIS		139	95.410	36.111	-0.065		20.00	7
	ATOM	553	CA	HIS	В	139	95.871	34.984	0.731		20.00	6
55	ATOM	554	CB	HIS	В	139	94.769	34.610	1.737		20.00	6
	MOTA	555	CG	HIS		139	95.173	33.561	2.725	1.00		6
	ATOM	556		HIS		139	95.543	33.657	4.025	1.00		6
	ATOM	557		HIS		139	95.241	32.221	2.405		20.00	7
	ATOM	558	CE1	HIS	В	139	95.635	31.537	3.466	1.00	20.00	6

	ATOM	559	NE2	HIS	В	139	95.825	32.385	4.461	1.00 20.00	7
	ATOM	560	С	HIS	В	139	96.176	33.828	-0.221	1.00 20.00	6
	ATOM	561	0	HIS	В	139	95.444	33.595	-1.182	1.00 20.00	8
	MOTA	562	N	PRO		140	97.257	33.080	0.038	1.00 20.00	
5	ATOM	563	CD	PRO		140	98.128	33.140	1.225	1.00 20.00	
	ATOM	564	CA	PRO		140	97.635	31.959	-0.827	1.00 20.00	
	ATOM	565	CB	PRO		140	98.913	31.433	-0.171	1.00 20.00	
	ATOM	566	CG	PRO		140	98.687	31.730	1.277	1.00 20.00	
	ATOM	567	C	PRO			96.614	30.846	-1.072	1.00 20.00	
10											
10	MOTA	568	0	PRO		140	96.747	30.107	-2.044	1.00 20.00	
	MOTA	569	N	PHE		141	95.607	30.712	-0.211	1.00 20.00	
	ATOM	570	CA	PHE			94.620	29.649	-0.398	1.00 20.00	
	MOTA	571	CB	PHE			94.206	29.056	0.961	1.00 20.00	
	ATOM	572	CG	PHE			95.321	28.335	1.681	1.00 20.00	
15	MOTA	573		PHE	В	141	96.351	27.716	0.967	1.00 20.00	
	ATOM	574	CD2	PHE	В	141	95.311	28.227	3.067	1.00 20.00	
	ATOM	575	CE1	PHE	В	141	97.350	27.000	1.627	1.00 20.00	6
	ATOM	576	CE2	PHE	В	141	96.307	27.510	3.740	1.00 20.00	6
	ATOM	577	CZ	PHE	В	141	97.328	26.895	3.018	1.00 20.00	6
20	ATOM	578	C	PHE	В	141	93.371	30.063	-1.181	1.00 20.00	6
	ATOM	579	0	PHE	В	141	92.335	29.398	-1.114	1.00 20.00	8
	ATOM	580	N	PHE	В	142	93.471	31.150	-1.934	1.00 20.00	
	ATOM	581	CA	PHE			92.337	31.625	-2.721	1.00 20.00	
	ATOM	582	CB			142	91.739	32.883	-2.082	1.00 20.00	
25	ATOM	583	CG	PHE			91.048	32.628	-0.772	1.00 20.00	
20	ATOM	584		PHE		142	89.715	32.227	-0.740	1.00 20.00	
	ATOM	585		PHE			91.741	32.747	0.429	1.00 20.00	
	ATOM	586		PHE		142	89.080	31.944	0.472	1.00 20.00	
	ATOM	587		PHE		142	91.116	32.465	1.647	1.00 20.00	
30	ATOM	588	CZ	PHE		142	89.785	32.463	1.667	1.00 20.00	
30		589	C	PHE			92.758	31.945	-4.146	1.00 20.00	
	ATOM										
	ATOM	590	0	PHE			93.865	32.429	-4.371	1.00 20.00	
	ATOM	591	N	VAL			91.883	31.653	-5.106	1.00 20.00	
	MOTA	592	CA	VAL		143	92.167	31.960	-6.504	1.00 20.00	
35	ATOM	593	CB	VAL		143	91.009	31.513	-7.435	1.00 20.00	
	ATOM	594		VAL		143	91.116	32.209	-8.795	1.00 20.00	
	ATOM	595	CG2	VAL		143	91.061	30.000	-7.623	1.00 20.00	
	ATOM	596	C	VAL		143	92.301	33.469	-6.545	1.00 20.00	
	ATOM	597	0	VAL		143	91.505	34.179	-5.932	1.00 20.00	
40	ATOM	598	N	LYS	В	144	93.312	33.957	-7.252	1.00 20.00	7
	ATOM	599	CA	LYS	В	144	93.547	35.392	-7.340	1.00 20.00	6
	MOTA	600	CB	LYS	В	144	95.051	35.689	-7.267	1.00 20.00	6
	ATOM	601	CG	LYS	В	144	95.382	37.182	-7.318	1.00 20.00	6
	ATOM	602	CD	LYS	В	144	96.881	37.441	-7.201	1.00 20.00	6
45	ATOM	603	CE	LYS	В	144	97.191	38.936	-7.298	1.00 20.00	6
	ATOM	604	NZ	LYS	В	144	98.661	39.215	-7.246	1.00 20.00	7
	ATOM	605	C	LYS		144	92.989	36.003	-8.614	1.00 20.00	
	ATOM	606	ō	LYS		144	92.993	35.371	-9.675	1.00 20.00	
	ATOM	607	N	LEU			92.495	37.230	-8.490	1.00 20.00	
50	ATOM	608	CA	LEU			91.968	37.975	-9.624	1.00 20.00	
50	ATOM	609	СВ	LEU			90.678	38.703	-9.234	1.00 20.00	
	ATOM	610	CG	LEU			89.938		-10.326	1.00 20.00	
	ATOM	611		LEU		145	88.611	39.992	-9.782	1.00 20.00	
	ATOM	612		LEU		145	90.791		-10.806	1.00 20.00	
55		613	CD2	LEU		145	93.059	38.984	-9.968	1.00 20.00	
33	ATOM										
	MOTA	614	0	LEU		145	93.291	39.940	-9.216	1.00 20.00	
	MOTA	615	N	TYR		146	93.735		-11.093	1.00 20.00	
	MOTA	616	CA	TYR		146	94.815		-11.517	1.00 20.00	
	ATOM	617	CB	TYR	В	146	95.821	38.904	-12.389	1.00 20.00	6

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	ATOM	618	CG	TYR			96.624 96.139	37.858 -11.661 36.559 -11.498	1.00 20.00	6
	MOTA	619		TYR		146				6
	ATOM	620		TYR		146	96.894	35.589 -10.836	1.00 20.00	6
5	MOTA	621	CD2	TYR		146	97.878	38.165 -11.140	1.00 20.00	6
3	ATOM	622	CE2	TYR		146	98.639	37.208 -10.476	1.00 20.00	6
	MOTA	623	CZ	TYR		146	98.144	35.925 -10.331	1.00 20.00	6
	ATOM	624	OH	TYR		146	98.920	34.981 -9.706	1.00 20.00	8
	ATOM	625	C	TYR		146	94.357	40.884 -12.293	1.00 20.00	6
10	MOTA	626	0	TYR		146	94.933	41.963 -12.160	1.00 20.00	8
10	MOTA	627	N	PHE		147	93.326	40.722 -13.110	1.00 20.00	7
	MOTA	628	CA			147	92.855	41.832 -13.923	1.00 20.00	6
	ATOM	629	CB	PHE		147	93.823	42.044 -15.092	1.00 20.00	6
	MOTA	630	CG	PHE			94.027	40.809 -15.945	1.00 20.00	6
1.5	MOTA	631		PHE			93.049	40.397 -16.850	1.00 20.00	6
15	MOTA	632	CD2				95.188	40.047 -15.822	1.00 20.00	6
	MOTA	633	CE1			147	93.221	39.247 -17.617	1.00 20.00	6
	MOTA	634	CE2	PHE			95.372	38.893 -16.585	1.00 20.00	6
	MOTA	635	CZ	PHE		147	94.388	38.490 -17.485	1.00 20.00	6
	MOTA	636	С	PHE			91.473	41.566 -14.480	1.00 20.00	6
20	MOTA	637	0	PHE			90.972	40.442 -14.423	1.00 20.00	8
	MOTA	638	N	THR			90.865	42.616 -15.021	1.00 20.00	7
	MOTA	639	CA	THR		148	89.560	42.509 -15.643	1.00 20.00	6
	MOTA	640	СВ	THR		148	88.402	42.889 -14.678	1.00 20.00	6
	MOTA	641		THR			88.492	44.275 -14.338	1.00 20.00	8
25	MOTA	642	CG2	THR		148	88.460	42.057 -13.403	1.00 20.00	6
	MOTA	643	C	THR		148	89.532	43.469 -16.821	1.00 20.00	6
	MOTA	644	0	THR		148	90.281	44.448 -16.866	1.00 20.00	8
	MOTA	645	N	PHE			88.685	43.161 -17.791	1.00 20.00	7
	MOTA	646	CA	PHE		149	88.508	44.011 -18.948	1.00 20.00	6
30	MOTA	647	CB	PHE		149	89.750	44.013 -19.864	1.00 20.00	6
	MOTA	648	CG	PHE		149	90.133	42.664 -20.419	1.00 20.00	6
	ATOM	649		PHE		149	89.552	42.182 -21.587	1.00 20.00	6
	MOTA	650		PHE			91.122	41.903 -19.802	1.00 20.00	6
	MOTA	651		PHE			89.953	40.965 -22.142	1.00 20.00	6
35	MOTA	652	CE2			149	91.532	40.681 -20.345	1.00 20.00	6
	ATOM	653	CZ	PHE		149	90.948	40.213 -21.517	1.00 20.00	6
	MOTA	654	C	PHE			87.271	43.498 -19.649	1.00 20.00	6
	MOTA	655	0	PHE			86.714	42.474 -19.251	1.00 20.00	8
	ATOM	656	N	GLN			86.812	44.221 -20.657	1.00 20.00	7
40	MOTA	657	CA	GLN			85.619	43.807 -21.372	1.00 20.00	6
	MOTA	658	CB	GLN			84.358	44.260 -20.614	1.00 20.00	6
	MOTA	659	CG	GLN			84.302	45.761 -20.289	1.00 20.00	6
	ATOM	660	CD	GLN			83.011	46.172 -19.567	1.00 20.00	6
	ATOM	661		GLN			81.970	46.385 -20.196	1.00 20.00	8
45	ATOM	662		GLN			83.078	46.273 -18.240	1.00 20.00	7
	MOTA	663	C	GLN			85.598	44.400 -22.760	1.00 20.00	6
	ATOM	664	0	GLN			86.281	45.387 -23.033	1.00 20.00	8
	MOTA	665	N	ASP			84.846	43.766 -23.649	1.00 20.00	7
	MOTA	666	CA	ASP			84.683	44.296 -24.992	1.00 20.00	6
50	MOTA	667	CB	ASP			85.160	43.312 -26.074	1.00 20.00	6
	MOTA	668	CG	ASP		151	84.558	41.934 -25.939	1.00 20.00	6
	MOTA	669		ASP			83.425	41.812 -25.436	1.00 20.00	8
	MOTA	670		ASP			85.227	40.963 -26.365	1.00 20.00	8
	ATOM	671	C	ASP			83.188	44.573 -25.095	1.00 20.00	6
55	MOTA	672	0	ASP			82.501	44.610 -24.069	1.00 20.00	8
	MOTA	673	N	ASP			82.669	44.758 -26.301	1.00 20.00	7
	MOTA	674	CA	ASP		152	81.251	45.062 -26.437	1.00 20.00	6
	ATOM	675	CB	ASP			80.907	45.346 -27.901	1.00 20.00	6
	ATOM	676	CG	ASP	В	152	81.616	46.574 -28.432	1.00 20.00	6

	ATOM	677	OD1	ASP	В	152	81.748	47.555 -27.666	1.00 20.00	8
	ATOM	678	OD2	ASP	В	152	82,030	46.563 -29.613	1.00 20.00	8
	ATOM	679	C	ASP			80.285	44.020 -25.888	1.00 20.00	6
	ATOM	680	ō	ASP			79.229	44.367 -25.357	1.00 20.00	8
5	ATOM	681	N	GLU			80.641	42.747 -25.982	1.00 20.00	7
	ATOM	682	CA	GLU			79.727	41.711 -25.521	1.00 20.00	6
	ATOM	683	CB	GLU			79.516	40.685 -26.641	1.00 20.00	6
	ATOM	684	CG	GLU			79.577	41.260 -28.058	1.00 20.00	6
	ATOM	685	CD	GLU			81.006	41.472 -28.550	1.00 20.00	6
10										
10	ATOM	686		GLU			81.765	40.480 -28.635	1.00 20.00	8
	MOTA	687	OE2	GLU			81.374	42.627 -28.854	1.00 20.00	8
	ATOM	688	C	GLU			80.102	40.960 -24.247	1.00 20.00	6
	ATOM	689	0	GLU			79.222	40.473 -23.535	1.00 20.00	8
	ATOM	690	N	LYS	В	154	81.393	40.869 -23.944	1.00 20.00	7
15	MOTA	691	CA	LYS	В	154	81.818	40.091 -22.787	1.00 20.00	6
	ATOM	692	CB	LYS	В	154	82.549	38.830 -23.273	1.00 20.00	6
	ATOM	693	CG	LYS	В	154	81.785	37.978 -24.278	1.00 20.00	6
	ATOM	694	CD	LYS	В	154	82.727	37.028 -25.021	1.00 20.00	6
	ATOM	695	CE	LYS	В	154	81.968	36.086 -25.952	1.00 20.00	6
20	ATOM	696	NZ	LYS	В	154	82.894	35.300 -26.826	1.00 20.00	7
	ATOM	697	C	LYS			82.709	40.767 -21.756	1.00 20.00	6
	ATOM	698	o	LYS			83.412	41.740 -22.048	1.00 20.00	8
	ATOM	699	N	LEU			82.677	40.202 -20.551	1.00 20.00	7
	ATOM	700	CA	LEU			83.501	40.638 -19.428	1.00 20.00	6
25	ATOM	701	CB	LEU			82.700	40.651 -18.127	1.00 20.00	6
23	ATOM	702	CG	LEU			81.451	41.521 -18.004	1.00 20.00	6
	ATOM	703		LEU			80.805	41.273 -16.645	1.00 20.00	6
	ATOM	704		LEU			81.831	42.983 -18.152	1.00 20.00	6
20	ATOM	705	С	LEU			84.578	39.559 -19.302	1.00 20.00	6
30	MOTA	706	0	LEU			84.288	38.379 -19.495	1.00 20.00	8
	MOTA	707	N	TYR			85.802	39.956 -18.966	1.00 20.00	7
	ATOM	708	CA	TYR			86.893	38.998 -18.809	1.00 20.00	6
	ATOM	709	CB	TYR			87.953	39.189 -19.904	1.00 20.00	6
	ATOM	710	CG	TYR			87.450	39.053 -21.324	1.00 20.00	6
35	MOTA	711		TYR			86.688	40.061 -21.920	1.00 20.00	6
	ATOM	712	CE1	TYR	В	156	86.233	39.938 -23.235	1.00 20.00	6
	ATOM	713	CD2	TYR	В	156	87.741	37.917 -22.077	1.00 20.00	6
	ATOM	714	CE2	TYR	В	156	87.288	37.782 -23.387	1.00 20.00	6
	ATOM	715	CZ	TYR	В	156	86.538	38.794 -23.958	1.00 20.00	6
40	MOTA	716	OH	TYR	В	156	86.087	38.656 -25.246	1.00 20.00	8
	ATOM	717	С	TYR	В	156	87.566	39.182 -17.447	1.00 20.00	6
	MOTA	718	0	TYR	В	156	87.977	40.291 -17.110	1.00 20.00	8
	ATOM	719	N	PHE			87.657	38.104 -16.667	1.00 20.00	7
	ATOM	720	CA	PHE			88.325	38.152 -15.367	1.00 20.00	6
45	ATOM	721	CB	PHE		157	87.448	37.575 -14.246	1.00 20.00	6
	ATOM	722	CG	PHE			86.194	38.360 -13.968	1.00 20.00	6
	ATOM	723		PHE			85.986	39.614 -14.535	1.00 20.00	6
	ATOM	724		PHE			85.206	37.828 -13.143	1.00 20.00	6
		725		PHE			84.808	40.324 -14.290	1.00 20.00	
50	MOTA									6
30	MOTA	726		PHE			84.025	38.532 -12.893	1.00 20.00	6
	MOTA	727	CZ	PHE			83.829	39.782 -13.470	1.00 20.00	6
	MOTA	728	C	PHE			89.579	37.295 -15.471	1.00 20.00	6
	MOTA	729	0	PHE			89.492	36.105 -15.765	1.00 20.00	8
	MOTA	730	N	GLY			90.742	37.893 -15.231	1.00 20.00	7
55	MOTA	731	CA	GLY			91.985	37.146 -15.303	1.00 20.00	6
	MOTA	732	C	GLY			92.254	36.512 -13.955	1.00 20.00	6
	MOTA	733	0	GLY		158	92.575	37.211 -12.996	1.00 20.00	8
	MOTA	734	N	LEU	В	159	92.137	35.191 -13.886	1.00 20.00	7
	ATOM	735	CA	LEU	В	159	92.330	34.466 -12.634	1.00 20.00	6

	ATOM	736	CB	LEU	В	159	91.116	33.580 -12.358	1.00 20.00	6
	ATOM	737	CG			159	89.724	34.208 -12.490	1.00 20.00	6
	ATOM	738		LEU			88.670	33.111 -12.398	1.00 20.00	6
	ATOM	739		LEU		159	89.513	35.246 -11.404	1.00 20.00	6
-										
5	MOTA	740	C	LEU			93.562	33.582 -12.643	1.00 20.00	6
	MOTA	741	0	LEU		159	94.061	33.204 -13.698	1.00 20.00	8
	MOTA	742	N	SER		160	94.046	33.237 -11.457	1.00 20.00	7
	MOTA	743	CA	SER	В	160	95.192	32.356 -11.377	1.00 20.00	6
	MOTA	744	CB	SER	В	160	95.665	32.206 -9.926	1.00 20.00	6
10	ATOM	745	OG	SER	В	160	94.591	31.973 -9.042	1.00 20.00	8
	ATOM	746	С	SER	В	160	94.754	31.012 -11.951	1.00 20.00	6
	ATOM	747	ō			160	93.598	30.605 -11.813	1.00 20.00	8
	ATOM	748	N	TYR			95.674	30.339 -12.625	1.00 20.00	7
	ATOM	749	CA	TYR			95.381	29.050 -13.231	1.00 20.00	6
15		750					96.170			
13	MOTA		CB	TYR		161		28.924 -14.543	1.00 20.00	6
	MOTA	751	CG	TYR		161	96.128	27.564 -15.209	1.00 20.00	6
	MOTA	752		TYR		161	94.968	26.787 -15.193	1.00 20.00	6
	ATOM	753		TYR		161	94.915	25.554 -15.846	1.00 20.00	6
	MOTA	754	CD2	TYR	В	161	97.240	27.073 -15.895	1.00 20.00	6
20	ATOM	755	CE2	TYR	В	161	97.198	25.841 -16.553	1.00 20.00	6
	ATOM	756	CZ	TYR	В	161	96.033	25.088 -16.523	1.00 20.00	6
	ATOM	757	OH	TYR	В	161	95.983	23.877 -17.173	1.00 20.00	8
	ATOM	758	С	TYR		161	95.724	27.905 -12.277	1.00 20.00	6
	ATOM	759	ō	TYR			96.897	27.598 -12.065	1.00 20.00	8
25	ATOM	760	N	ALA		162	94.696	27.288 -11.697	1.00 20.00	7
23		761	CA	ALA			94.893	26.166 -10.776	1.00 20.00	6
	ATOM									
	MOTA	762	CB	ALA		162	93.666	25.995 -9.873	1.00 20.00	6
	MOTA	763	C	ALA			95.100	24.924 -11.637	1.00 20.00	6
	MOTA	764	0	ALA		162	94.146	24.251 -12.015		8
30	MOTA	765	N	LYS		163	96.361	24.626 -11.930	1.00 20.00	7
	MOTA	766	CA	LYS	В	163	96.722	23.506 -12.795		6
	ATOM	767	CB	LYS	В	163	98.247	23.416 -12.912	1.00 20.00	6
	ATOM	768	CG	LYS	В	163	98.904	24.711 -13.360	1.00 20.00	6
	ATOM	769	CD	LYS	В	163	100.405	24.539 -13.554	1.00 20.00	6
35	ATOM	770	CE	LYS	В	163	101.102	25.885 -13.690	1.00 20.00	6
	ATOM	771	NZ	LYS			100.976	26.701 -12.445	1.00 20.00	7
	ATOM	772	C	LYS			96.170	22.123 -12.464	1.00 20.00	6
	ATOM	773	Ö	LYS		163	95.823	21.370 -13.369	1.00 20.00	8
	ATOM	774	N	ASN		164	96.076	21.775 -11.186	1.00 20.00	7
40										
40	MOTA	775	CA	ASN		164	95.594	20.449 -10.842	1.00 20.00	6
	MOTA	776	CB	ASN		164	96.339	19.944 -9.610	1.00 20.00	6
	MOTA	777	CG	ASN		164	97.766	19.529 -9.943	1.00 20.00	6
	MOTA	778		ASN		164	97.992	18.776 -10.892	1.00 20.00	8
	MOTA	779	ND2	ASN	В	164	98.730	20.014 -9.171	1.00 20.00	7
45	ATOM	780	C	ASN	В	164	94.084	20.246 -10.706	1.00 20.00	6
	ATOM	781	0	ASN	В	164	93.630	19.183 -10.286	1.00 20.00	8
	ATOM	782	N	GLY	В	165	93.309	21.257 -11.080	1.00 20.00	7
	ATOM	783	CA	GLY		165	91.863	21.127 -11.039	1.00 20.00	6
	ATOM	784	C	GLY			91.159	21.088 -9.694	1.00 20.00	6
50	ATOM	785	ō	GLY			91.663	21.598 -8.698	1.00 20.00	
50	ATOM	786	N	GLU			89.986	20.461 -9.689	1.00 20.00	7
	ATOM	787	CA	GLU		166	89.126	20.344 -8.513		6
	MOTA	788	СВ	GLU		166	87.683	20.079 -8.962	1.00 20.00	6
	MOTA	789	CG	GLU		166	86.992	21.255 -9.646		6
55	MOTA	790	CD	GLU		166	85.709	20.837 -10.358	1.00 20.00	6
	MOTA	791		GLU		166	85.137	19.794 -9.986		8
	MOTA	792	OE2			166	85.263	21.556 -11.279	1.00 20.00	8
	MOTA	793	C	GLU	В	166	89.520	19.270 -7.506	1.00 20.00	6
	MOTA	794	0	GLU	В	166	89.952	18.184 -7.874	1.00 20.00	8

	MOTA	795	N	LEU			89.344	19.579	-6.226		20.00	7
	MOTA	796	CA	LEU	В	167	89.651	18.626	-5.168	1.00	20.00	6
	MOTA	797	CB	LEU	В	167	89.395	19.269	-3.802	1.00	20.00	6
	MOTA	798	CG	LEU	В	167	89.408	18.363	-2.569	1.00	20.00	6
5	ATOM	799	CD1	LEU	В	167	90.769	17.703	-2.412	1.00	20.00	6
	MOTA	800	CD2	LEU	В	167	89.065	19.193	-1.338	1.00	20.00	6
	ATOM	801	С	LEU		167	88.757	17.394	-5.346		20.00	6
	ATOM	802	ō	LEU		167	89.124	16.283	-4.968		20.00	8
	ATOM	803	N	LEU		168	87.580	17.600	-5.927		20.00	7
10	ATOM	804	CA	LEU		168	86.647	16.500	-6.153		20.00	6
	ATOM	805	CB	LEU		168	85.364	17.014	-6.809		20.00	6
	ATOM	806	CG	LEU		168	84.292	15.977	-7.168		20.00	6
	ATOM	807		LEU		168	83.883	15.186	-5.929		20.00	6
		808		LEU		168	83.083	16.687	-7.756		20.00	
	ATOM											6
15	ATOM	809	С	LEU		168	87.290	15.440	-7.046		20.00	6
	MOTA	810	0	LEU		168	87.091	14.243	-6.845		20.00	8
	MOTA	811	N	LYS		169	88.068	15.888	-8.027		20.00	7
	MOTA	812	CA	LYS		169	88.727	14.967	-8.941		20.00	6
	MOTA	813	CB	LYS		169	89.610	15.729	-9.930		20.00	6
20	MOTA	814	CG	LYS		169	90.379		-10.882		20.00	6
	ATOM	815	CD	LYS	В	169	91.226	15.603	-11.877	1.00	20.00	6
	MOTA	816	CE	LYS	В	169	92.373	16.328	-11.192	1.00	20.00	6
	MOTA	817	NZ	LYS	В	169	93.253	17.021	-12.173	1.00	20.00	7
	ATOM	818	C	LYS	В	169	89.574	13.949	-8.193	1.00	20.00	6
25	ATOM	819	0	LYS	В	169	89.543	12.758	-8.504	1.00	20.00	8
	ATOM	820	N	TYR	В	170	90.334	14.417	-7.207	1.00	20.00	7
	ATOM	821	CA	TYR	В	170	91.197	13.527	-6.441	1.00	20.00	6
	ATOM	822	CB	TYR	В	170	92.243	14.346	-5.682	1.00	20.00	6
	ATOM	823	CG	TYR	В	170	93.217	15.010	-6.624	1.00	20.00	6
30	ATOM	824		TYR		170	94.347	14.331	-7.085		20.00	6
	ATOM	825		TYR		170	95.195	14.900	-8.036		20.00	6
	ATOM	826	CD2			170	92.963	16.282	-7.133		20.00	6
	ATOM	827	CE2	TYR		170	93.801	16.861	-8.083		20.00	6
	ATOM	828	CZ	TYR		170	94.913	16.164	-8.532		20.00	6
35	ATOM	829	OH	TYR		170	95.727	16.727	-9.493		20.00	8
33	ATOM	830	C	TYR		170	90.419	12.622	-5.499		20.00	6
			o									8
	ATOM	831		TYR		170	90.834	11.494	-5.233		20.00	
	ATOM	832	N	ILE		171	89.287	13.098	-4.993		20.00	7
40	ATOM	833	CA	ILE		171	88.488	12.262	-4.112		20.00	6
40	MOTA	834	CB	ILE			87.278	13.028	-3.538		20.00	6
	MOTA	835		ILE		171	86.367	12.065	-2.791		20.00	6
	MOTA	836		ILE		171	87.764	14.141	-2.603		20.00	6
	ATOM	837		ILE			86.652	14.990	-2.019		20.00	6
	MOTA	838	С	ILE		171	87.994	11.066	-4.931		20.00	6
45	ATOM	839	0	ILE	В	171	88.030	9.925	-4.468	1.00	20.00	8
	MOTA	840	N	ARG	В	172	87.550	11.331	-6.156	1.00	20.00	7
	MOTA	841	CA	ARG	В	172	87.061	10.273	-7.031	1.00	20.00	6
	ATOM	842	CB	ARG	В	172	86.359	10.861	-8.259	1.00	20.00	6
	ATOM	843	CG	ARG	В	172	85.094	11.658	-7.963	1.00	20.00	6
50	MOTA	844	CD	ARG	В	172	84.352	11.981	-9.259	1.00	20.00	6
	MOTA	845	NE	ARG	В	172	83.187	12.843	-9.063	1.00	20.00	7
	MOTA	846	CZ	ARG	В	172	82.192	12.589	-8.217	1.00	20.00	6
	ATOM	847		ARG		172	82.209	11.491	-7.469		20.00	7
	ATOM	848		ARG		172	81.168	13.428	-8.127	1.00		7
55	ATOM	849	C	ARG		172	88.202	9.378	-7.497	1.00		6
22	ATOM	850	0	ARG		172	88.050	8.160	-7.587	1.00		8
	ATOM	851	N	LYS		173	89.348	9.985	-7.783		20.00	7
							90.509					
	MOTA	852	CA	LYS		173		9.244	-8.256		20.00	6
	MOTA	853	CB	LYS	В	173	91.647	10.206	-8.603	T.00	20.00	6

	ATOM	854	CG			173	92.930	9.511	-9.045	1.00		6
	ATOM	855	CD	LYS		173	94.081	10.496	-9.222	1.00		6
	MOTA	856	CE	LYS	В	173	93.862	11.432	-10.406	1.00	20.00	6
	MOTA	857	NZ	LYS	В	173	93.858	10.711	-11.715	1.00	20.00	7
5	ATOM	858	C	LYS	В	173	91.025	8.191	-7.280	1.00	20.00	6
	ATOM	859	0	LYS	В	173	91.274	7.055	-7.674	1.00	20.00	8
	ATOM	860	N	ILE	В	174	91.192	8.554	-6.012	1.00	20.00	7
	ATOM	861	CA	ILE	В	174	91.710	7.593	-5.042	1.00	20.00	6
	ATOM	862	CB	ILE	В	174	92.884	8.191	-4.223	1.00	20.00	6
10	ATOM	863	CG2	ILE	В	174	93.970	8.701	-5.166	1.00	20.00	6
	ATOM	864		ILE		174	92.394	9.337	-3.343	1.00		6
	ATOM	865				174	93.480	9.916	-2.457	1.00		6
	ATOM	866	С	ILE	В	174	90.674	7.030	-4.074	1.00		6
	ATOM	867	ō	ILE		174	91.025	6.296	-3.151	1.00		8
15	ATOM	868	N	GLY		175	89.405	7.367	-4.283	1.00		7
	ATOM	869	CA	GLY		175	88.359	6.855	-3.413	1.00		6
	ATOM	870	C	GLY			88.160	7.650	-2.138	1.00		6
	ATOM	871	ŏ	GLY		175	87.083	8.198	-1.905	1.00		8
	ATOM	872	N	SER		176	89.192	7.701	-1.304	1.00		7
20	ATOM	873	CA	SER		176	89.140	8.447	-0.053	1.00		6
20	ATOM	874	CB	SER		176	88.395	7.653	1.026	1.00		6
	ATOM	875	OG	SER		176	89.150	6.543	1.472	1.00		8
	ATOM	876	C	SER		176	90.565	8.742	0.401	1.00		6
	ATOM	877	0	SER			91.506	8.049	0.009	1.00		8
25						177	90.718	9.769	1.228			7
23	ATOM	878 879	N	PHE			92.029		1.722	1.00		
	ATOM		CA	PHE	В	177		10.184	1.722	1.00		6
	ATOM	880	CB	PHE		177	92.028 92.002	11.694	0.747	1.00		6
	ATOM	881	CG	PHE	В	177				1.00		6
20	MOTA	882		PHE		177	91.484	12.060	-0.449	1.00		6
30	ATOM	883	CD2	PHE	В	177	92.481	13.855	0.787	1.00		6
	ATOM	884	CE1			177	91.443	12.860	-1.585	1.00		6
	MOTA	885	CE2	PHE		177	92.444	14.665	-0.343	1.00		6
	MOTA	886	CZ	PHE			91.925	14.168	-1.532	1.00		6
	MOTA	887	C	PHE		177	92.427	9.475	3.009	1.00		6
35	MOTA	888	0	PHE		177	91.582	9.223	3.872	1.00		8
	MOTA	889	N	ASP		178	93.711	9.152	3.147	1.00		7
	MOTA	890	CA	ASP		178	94.155	8.529	4.385	1.00		6
	MOTA	891	CB	ASP		178	95.581	7.972	4.267	1.00		6
	MOTA	892	CG	ASP			96.594	9.018	3.845	1.00		6
40	MOTA	893		ASP			96.392	10.214	4.139	1.00		8
	MOTA	894		ASP			97.612	8.634	3.230	1.00		8
	MOTA	895	C	ASP		178	94.092	9.640	5.436	1.00		6
	MOTA	896	0	ASP			93.736	10.778	5.117	1.00		8
	MOTA	897	N	GLU			94.443	9.324	6.677	1.00		7
45	MOTA	898	CA	GLU			94.380	10.311	7.744	1.00		6
	ATOM	899	CB	GLU		179	94.623	9.637	9.096	1.00		6
	ATOM	900	CG	GLU		179	94.747	10.611	10.255	1.00		6
	MOTA	901	CD	GLU			94.331	9.994	11.574	1.00		6
	MOTA	902		GLU	В	179	94.589	8.789	11.770	1.00	20.00	8
50	MOTA	903	OE2	GLU	В	179	93.753	10.717	12.416	1.00	20.00	8
	MOTA	904	C	GLU	В	179	95.320	11.501	7.575	1.00	20.00	6
	MOTA	905	0	GLU	В	179	94.948	12.636	7.881	1.00	20.00	8
	MOTA	906	N	THR		180	96.528	11.246	7.086	1.00		7
	MOTA	907	CA	THR	В	180	97.509	12.308	6.886	1.00	20.00	6
55	MOTA	908	CB	THR	В	180	98.866	11.720	6.445	1.00	20.00	6
	MOTA	909	OG1	THR	В	180	99.349	10.842	7.466	1.00	20.00	8
	ATOM	910	CG2	THR	В	180	99.888	12.825	6.213	1.00	20.00	6
	ATOM	911	C	THR	В	180	97.040	13.331	5.849	1.00	20.00	6
	MOTA	912	0	THR	В	180	97.136	14.542	6.069	1.00	20.00	8

	ATOM	913	N	CYS	В	181	96.534	12.845	4.721	1.00 2	0.00	7
	ATOM	914	CA	CYS	В	181	96.057	13.733	3.666	1.00 2	0.00	6
	ATOM	915	CB	CYS	В	181	95.836	12.945	2.375	1.00 2	0.00	6
	ATOM	916	SG	CYS		181	97.372	12,255	1.685	1.00 2		16
5	ATOM	917	C	CYS		181	94.775	14.449	4.079	1.00 2		6
	ATOM	918	ŏ	CYS			94.570	15.615	3.733	1.00 2		8
	ATOM	919	N	THR			93.914	13.755	4.820	1.00 2		7
	ATOM	920	CA	THR			92.669	14.356	5.286	1.00 2		6
	ATOM	921	CB	THR			91.812	13.354	6.103	1.00 2		6
10	ATOM	922		THR			91.372	12.283	5.259	1.00 2		8
10												
	ATOM	923	CG2	THR		182	90.600	14.054	6.690	1.00 2		6
	ATOM	924	С	THR			93.014	15.535	6.196	1.00 2		6
	MOTA	925	0	THR			92.515	16.649	6.019	1.00 2		8
	MOTA	926	N	ARG			93.873	15.273	7.175	1.00 2		7
15	MOTA	927	CA	ARG			94.299	16.293	8.121	1.00 2		6
	MOTA	928	CB	ARG			95.311	15.707	9.109	1.00 2		6
	MOTA	929	CG	ARG			95.957	16.744	10.012	1.00 2		6
	ATOM	930	CD	ARG	В	183	96.886	16.116	11.050	1.00 2	0.00	6
	MOTA	931	NE	ARG	В	183	96.167	15.220	11.949	1.00 2	0.00	7
20	MOTA	932	CZ	ARG	В	183	96.098	13.900	11.804	1.00 2	0.00	6
	ATOM	933	NH1	ARG	В	183	96.717	13.306	10.791	1.00 2	0.00	7
	MOTA	934	NH2	ARG	В	183	95.389	13.176	12.664	1.00 2	0.00	7
	ATOM	935	C	ARG	В	183	94.923	17.505	7.427	1.00 2	0.00	6
	ATOM	936	0	ARG	В	183	94.545	18.646	7.698	1.00 2	0.00	8
25	ATOM	937	N	PHE	В	184	95.877	17.264	6.534	1.00 2	0.00	7
	ATOM	938	CA	PHE	В	184	96.539	18.367	5.847	1.00 2	0.00	6
	ATOM	939	CB	PHE			97.610	17.847	4.889	1.00 2		6
	ATOM	940	CG	PHE	В	184	98.387	18.943	4.223	1.00 2	0.00	6
	ATOM	941		PHE			99.451	19.555	4.879	1.00 2		6
30	ATOM	942		PHE			98.009	19.415	2.975	1.00 2		6
	ATOM	943		PHE			100.125	20.627	4.301	1.00 2		6
	ATOM	944		PHE			98.676	20.491	2.388	1.00 2		6
	ATOM	945	CZ	PHE			99.735	21.097	3.053	1.00 2		6
	ATOM	946	C	PHE			95.580	19.267	5.066	1.00 2		6
35	ATOM	947	Ö	PHE			95.567	20.481	5.255	1.00 2		8
33	ATOM	948	N	TYR			94.784	18.679	4.181	1.00 2		7
	ATOM	949	CA	TYR			93.854	19.471	3.390	1.00 2		6
	MOTA	950	CB	TYR			93.305	18.634	2.236	1.00 2		6
40	MOTA	951	CG	TYR			94.337	18.504	1.140	1.00 2		6
40	MOTA	952		TYR			94.611	19.580	0.293	1.00 2		6
	MOTA	953		TYR			95.637	19.516	-0.643	1.00 2		6
	MOTA	954	CD2	TYR			95.118	17.352	1.017	1.00 2		6
	MOTA	955	CE2				96.152	17.282	0.081	1.00 2		6
	MOTA	956	CZ	TYR			96.405	18.367	-0.742	1.00 2		6
45	MOTA	957	OH	TYR			97.436	18.314	-1.657	1.00 2		8
	MOTA	958	C	TYR			92.738	20.098	4.208	1.00 2		6
	ATOM	959	0	TYR			92.286	21.195	3.891	1.00 2		8
	MOTA	960	N	THR			92.303	19.422	5.267	1.00 2		7
	MOTA	961	CA	THR			91.265	19.987	6.122	1.00 2		6
50	MOTA	962	CB	THR	В	186	90.799	18.996	7.219	1.00 2	0.00	6
	MOTA	963	OG1	THR	В	186	90.193	17.846	6.606	1.00 2	0.00	8
	MOTA	964	CG2	THR	В	186	89.774	19.671	8.144	1.00 2	0.00	6
	MOTA	965	C	THR	В	186	91.858	21.218	6.805	1.00 2	0.00	6
	ATOM	966	0	THR	В	186	91.188	22.242	6.948	1.00 2	0.00	8
55	ATOM	967	N	ALA	В	187	93.120	21.115	7.222	1.00 2	0.00	7
	ATOM	968	CA	ALA	В	187	93.787	22.234	7.882	1.00 2	0.00	6
	ATOM	969	CB	ALA	В	187	95.184	21.817	8.349	1.00 2	0.00	6
	ATOM	970	C	ALA	В		93.879	23.449	6.946	1.00 2	0.00	6
	ATOM	971	0	ALA	В	187	93.654	24.585	7.372	1.00 2	0.00	8

	MOTA	972	N	GLU			94.205	23.222	5.674	1.00 20.00	7
	MOTA	973	CA	GLU		188	94.292	24.343	4.740	1.00 20.00	6
	MOTA	974	CB	GLU		188	94.843	23.898	3.376	1.00 20.00	6
	MOTA	975	CG	GLU		188	96.285	23.391	3.407	1.00 20.00	6
5	MOTA	976	CD	GLU		188	97.030	23.639	2.104	1.00 20.00	6
	MOTA	977		GLU		188	96.407	23.537	1.024	1.00 20.00	8
	MOTA	978	OE2	GLU		188	98.247	23.932	2.156	1.00 20.00	8
	MOTA	979	С	GLU		188	92.912	24.977	4.561	1.00 20.00	6
	MOTA	980	0	GLU		188	92.782	26.196	4.533	1.00 20.00	8
10	MOTA	981	N	ILE		189	91.875	24.152	4.451	1.00 20.00	7
	MOTA	982	CA	ILE	В	189	90.530	24.693	4.284	1.00 20.00	6
	MOTA	983	CB	ILE		189	89.495	23.566	4.064	1.00 20.00	6
	MOTA	984		ILE		189	88.094	24.157	3.947	1.00 20.00	6
	MOTA	985		ILE		189	89.855	22.773	2.796	1.00 20.00	6
15	MOTA	986		ILE		189	89.058	21.488	2.616	1.00 20.00	6
	MOTA	987	C	ILE			90.152	25.517	5.519	1.00 20.00	6
	MOTA	988	0	ILE			89.634	26.630	5.396	1.00 20.00	8
	MOTA	989	N	VAL		190	90.412	24.971	6.707	1.00 20.00	7
	MOTA	990	CA	VAL		190	90.116	25.674	7.957	1.00 20.00	6
20	MOTA	991	CB	VAL		190	90.557	24.842	9.186	1.00 20.00	6
	MOTA	992	CG1	VAL		190	90.540	25.717	10.451	1.00 20.00	6
	MOTA	993	CG2	VAL	В	190	89.643	23.641	9.358	1.00 20.00	6
	MOTA	994	C	VAL	В	190	90.865	27.012	7.984	1.00 20.00	6
	MOTA	995	0	VAL	В	190	90.311	28.039	8.375	1.00 20.00	8
25	MOTA	996	N	SER	В	191	92.125	26.997	7.557	1.00 20.00	7
	MOTA	997	CA	SER	В	191	92.934	28.218	7.546	1.00 20.00	6
	MOTA	998	CB	SER	В	191	94.378	27.888	7.166	1.00 20.00	6
	MOTA	999	OG	SER	В	191	95.220	29.007	7.363	1.00 20.00	8
	MOTA	1000	C	SER	В	191	92.361	29.240	6.566	1.00 20.00	6
30	MOTA	1001	0	SER	В	191	92.351	30.444	6.838	1.00 20.00	8
	MOTA	1002	N	ALA	В	192	91.882	28.754	5.425	1.00 20.00	7
	ATOM	1003	CA	ALA	В	192	91.306	29.634	4.417	1.00 20.00	6
	MOTA	1004	CB	ALA	В	192	91.006	28.850	3.141	1.00 20.00	6
	MOTA	1005	C	ALA	В	192	90.029	30.256	4.970	1.00 20.00	6
35	ATOM	1006	0	ALA	В	192	89.799	31.458	4.822	1.00 20.00	8
	MOTA	1007	N	LEU	В	193	89.203	29.439	5.621	1.00 20.00	7
	MOTA	1008	CA	LEU	В	193	87.957	29.941	6.192	1.00 20.00	6
	MOTA	1009	CB	LEU	В	193	87.101	28.783	6.725	1.00 20.00	6
	ATOM	1010	CG	LEU	В	193	86.447	27.898	5.650	1.00 20.00	6
40	ATOM	1011	CD1	LEU	В	193	85.645	26.771	6.315	1.00 20.00	6
	MOTA	1012	CD2	LEU	В	193	85.530	28.752	4.780	1.00 20.00	6
	MOTA	1013	C	LEU	В	193	88.215	30.959	7.299	1.00 20.00	6
	ATOM	1014	0	LEU	В	193	87.474	31.935	7.435	1.00 20.00	8
	MOTA	1015	N	GLU	В	194	89.254	30.738	8.100	1.00 20.00	7
45	ATOM	1016	CA	GLU	В	194	89.562	31.699	9.157	1.00 20.00	6
	MOTA	1017	CB	GLU	В	194	90.773	31.257	9.982	1.00 20.00	6
	ATOM	1018	CG	GLU	В	194	91.288	32.353	10.914	1.00 20.00	6
	ATOM	1019	CD	GLU	В	194	92.381	31.878	11.855	1.00 20.00	6
	ATOM	1020	OE1	GLU	В	194	93.246	31.090	11.420	1.00 20.00	8
50	ATOM	1021	OE2	GLU	В	194	92.376	32.312	13.031	1.00 20.00	8
	MOTA	1022	C	GLU	В	194	89.847	33.053	8.511	1.00 20.00	6
	MOTA	1023	0	GLU	В	194	89.375	34.083	8.972	1.00 20.00	8
	ATOM	1024	N	TYR	В	195	90.608	33.046	7.426	1.00 20.00	7
	ATOM	1025	CA	TYR	В	195	90.928	34.294	6.743	1.00 20.00	6
55	ATOM	1026	CB	TYR	В	195	91.919	34.043	5.613	1.00 20.00	6
	ATOM	1027	CG	TYR			92.193	35.271	4.774	1.00 20.00	6
	MOTA	1028	CD1	TYR	В	195	93.098	36.244	5.202	1.00 20.00	6
	MOTA	1029	CE1	TYR	В	195	93.356	37.382	4.429	1.00 20.00	6
	MOTA	1030	CD2	TYR	В	195	91.545	35.461	3.553	1.00 20.00	6

	ATOM	1031	CE2	TYR	В	195	91.794	36.591	2.775	1.00	20.00	6
	ATOM	1032	CZ	TYR	В	195	92.701	37.545	3.219	1.00	20.00	6
	ATOM	1033	OH	TYR	В	195	92.956	38.656	2.450	1.00	20.00	8
	ATOM	1034	C	TYR		195	89.668	34.923	6.160		20.00	6
5												
3	ATOM	1035	0	TYR		195	89.409	36.117	6.328		20.00	8
	MOTA	1036	N	LEU		196	88.885	34.103	5.472		20.00	7
	ATOM	1037	CA	LEU	В	196	87.664	34.576	4.845		20.00	6
	MOTA	1038	CB	LEU	В	196	86.972	33.426	4.107	1.00	20.00	6
	ATOM	1039	CG	LEU	В	196	85.933	33.824	3.060	1.00	20.00	6
10	ATOM	1040	CD1	LEU	В	196	86.602	34.659	1.966	1.00	20.00	6
	ATOM	1041	CD2	LEU			85.305	32.568	2.463		20.00	6
	ATOM	1042	C	LEU		196	86.731	35.161	5.888		20.00	6
	MOTA	1043	0	LEU		196	86.299	36.308	5.774		20.00	8
	ATOM	1044	N	HIS		197	86.431	34.378	6.917		20.00	7
15	MOTA	1045	CA	HIS	В	197	85.533	34.840	7.967	1.00	20.00	6
	ATOM	1046	CB	HIS	В	197	85.241	33.697	8.942	1.00	20.00	6
	ATOM	1047	CG	HIS	В	197	84.377	32.622	8.356	1.00	20.00	6
	ATOM	1048	CD2	HIS	В	197	83.734	32.550	7.163	1.00	20.00	6
	ATOM	1049		HIS		197	84.083	31.452	9.022		20.00	7
20	ATOM	1050		HIS	В	197	83.296	30.704	8.264		20.00	6
20	ATOM	1051				197	83.071	31.346	7.132		20.00	7
	MOTA	1052	С	HIS		197	86.080	36.060	8.697		20.00	6
	ATOM	1053	0	HIS		197	85.314	36.919	9.146		20.00	8
	MOTA	1054	N	GLY		198	87.404	36.143	8.804	1.00	20.00	7
25	ATOM	1055	CA	GLY	В	198	88.009	37.285	9.464	1.00	20.00	6
	ATOM	1056	C	GLY	В	198	87.687	38.580	8.737	1.00	20.00	6
	ATOM	1057	0	GLY	В	198	87.784	39.661	9.311	1.00	20.00	8
	ATOM	1058	N			199	87.308	38.475	7.466		20.00	7
	ATOM	1059	CA	LYS		199	86.959	39.652	6.674		20.00	6
30	ATOM	1060	CB		В	199	87.577	39.573	5.279		20.00	6
30												
	ATOM	1061	CG	LYS		199	89.082	39.736	5.258		20.00	6
	ATOM	1062	CD	LYS		199	89.574	39.919	3.833		20.00	6
	MOTA	1063	CE	LYS		199	91.054	40.243	3.807		20.00	6
	MOTA	1064	NZ	LYS	В	199	91.398	41.382	4.706	1.00	20.00	7
35	ATOM	1065	C	LYS	В	199	85.451	39.804	6.539	1.00	20.00	6
	ATOM	1066	0	LYS	В	199	84.972	40.556	5.693	1.00	20.00	8
	ATOM	1067	N	GLY	В	200	84.707	39.079	7.368	1.00	20.00	7
	ATOM	1068	CA	GLY		200	83.258	39.158	7.328		20.00	6
	ATOM	1069	C	GLY		200	82.646	38.660	6.032		20.00	6
40	ATOM	1070	Ö	GLY		200	81.644	39.198	5.564		20.00	8
40												
	MOTA	1071	N	ILE			83.243	37.630	5.445		20.00	7
	MOTA	1072	CA	ILE		201	82.726	37.075	4.205		20.00	6
	MOTA	1073	CB	ILE			83.775	37.140	3.080	1.00	20.00	6
	MOTA	1074	CG2	ILE	В	201	83.257	36.413	1.841	1.00	20.00	6
45	MOTA	1075	CG1	ILE	В	201	84.109	38.599	2.761	1.00	20.00	6
	ATOM	1076	CD1	ILE	В	201	85.330	38.758	1.870	1.00	20.00	6
	ATOM	1077	С	ILE	В	201	82.329	35.623	4.395	1.00	20.00	6
	ATOM	1078	ō	ILE		201	83.094	34.826	4.942		20.00	8
	ATOM	1079	N	ILE		202	81.125	35.291	3.940		20.00	7
50	ATOM	1080	CA	ILE		202	80.592	33.936	4.016		20.00	6
30												
	MOTA	1081	СВ		В	202	79.119	33.953	4.481		20.00	6
	MOTA	1082		ILE		202	78.583	32.522	4.595		20.00	6
	MOTA	1083	CG1	ILE	В	202	79.008	34.675	5.825	1.00	20.00	6
	ATOM	1084	CD1	ILE	В	202	77.576	34.865	6.294	1.00	20.00	6
55	MOTA	1085	C	ILE	В	202	80.644	33.393	2.589	1.00	20.00	6
	ATOM	1086	0	ILE	В	202	80.182	34.056	1.663	1.00	20.00	8
	ATOM	1087	N	HIS		203	81.204	32.204	2.395		20.00	7
	ATOM	1088	CA	HIS		203	81.279	31.652	1.044		20.00	6
	ATOM	1089	CB	HIS			82.258	30.480	0.999		20.00	6
	AIUM	1007	CD	1113	Д	203	02.230	50.400	0.555	1.00	20.00	0

	MOTA	1090	CG	HIS	В	203	82.478	29.942	-0.380	1.00 20.00	6
	MOTA	1091	CD2	HIS	В	203	81.646	29.282	-1.220	1.00 20.00	6
	MOTA	1092	ND1	HIS	В	203	83.659	30.116	-1.069	1.00 20.00	7
	MOTA	1093	CE1	HIS	В	203	83.545	29.588	-2.275	1.00 20.00	6
5	ATOM	1094	NE2	HIS	В	203	82.333	29.076	-2.392	1.00 20.00	7
	MOTA	1095	C	HIS	В	203	79.896	31.211	0.530	1.00 20.00	6
	ATOM	1096	ō	HIS			79.508	31.546	-0.593	1.00 20.00	8
	ATOM	1097	N	ARG			79.168	30.458	1.357	1.00 20.00	7
	ATOM	1098	CA	ARG			77.819	29.969	1.039	1.00 20.00	6
10	ATOM	1099	CB	ARG			76.916	31.117	0.583	1.00 20.00	6
	ATOM	1100	CG	ARG			76.601	32.120	1.675	1.00 20.00	6
	ATOM	1101	CD	ARG			75.316	32.878	1.377	1.00 20.00	6
	ATOM	1102	NE	ARG			75.376	33.616	0.119	1.00 20.00	7
	ATOM	1102	CZ	ARG			74.423	34.443	-0.303	1.00 20.00	6
15	ATOM	1103		ARG			73.336	34.636	0.436	1.00 20.00	7
13	ATOM	1104	NH2	ARG			74.555	35.084	-1.457	1.00 20.00	7
	ATOM	1106	С	ARG			77.700	28.829	0.030	1.00 20.00	6
	ATOM	1107	0	ARG			76.611	28.300	-0.177	1.00 20.00	8
20	ATOM	1108	N	ASP			78.792	28.456	-0.620	1.00 20.00	7
20	MOTA	1109	CA	ASP		205	78.718	27.342	-1.550	1.00 20.00	6
	MOTA	1110	CB	ASP		205	78.380	27.829	-2.961	1.00 20.00	6
	MOTA	1111	CG	ASP		205	77.941	26.694	-3.867	1.00 20.00	6
	MOTA	1112		ASP			77.544	25.638	-3.330	1.00 20.00	8
	MOTA	1113		ASP		205	77.982	26.853	-5.104	1.00 20.00	8
25	MOTA	1114	C	ASP		205	80.019	26.560	-1.547	1.00 20.00	6
	MOTA	1115	0	ASP		205	80.508	26.122	-2.588	1.00 20.00	8
	MOTA	1116	N	LEU			80.573	26.375	-0.354	1.00 20.00	7
	MOTA	1117	CA	LEU	В	206	81.819	25.652	-0.208	1.00 20.00	6
	MOTA	1118	CB	LEU	В	206	82.361	25.826	1.212	1.00 20.00	6
30	MOTA	1119	CG	LEU	В	206	83.764	25.271	1.471	1.00 20.00	6
	MOTA	1120	CD1	LEU	В	206	84.765	25.969	0.561	1.00 20.00	6
	ATOM	1121	CD2	LEU	В	206	84.135	25.477	2.933	1.00 20.00	6
	MOTA	1122	C	LEU	В	206	81.609	24.174	-0.514	1.00 20.00	6
	ATOM	1123	0	LEU	В	206	80.691	23.549	0.011	1.00 20.00	8
35	ATOM	1124	N	LYS	В	207	82.461	23.628	-1.375	1.00 20.00	7
	ATOM	1125	CA	LYS	В	207	82.379	22.223	-1.765	1.00 20.00	6
	ATOM	1126	СВ	LYS			81.160	22.000	-2.679	1.00 20.00	6
	ATOM	1127	CG	LYS			81.130	22.913	-3.893	1.00 20.00	6
	ATOM	1128	CD	LYS			79.876	22.720	-4.736	1.00 20.00	6
40	ATOM	1129	CE	LYS			79.788	23.797	-5.813	1.00 20.00	6
	ATOM	1130	NZ	LYS		207	78.695	23.557	-6.791	1.00 20.00	7
	ATOM	1131	c	LYS			83.657	21.808	-2.487	1.00 20.00	6
	ATOM	1132	ō	LYS			84.416	22.656	-2.960	1.00 20.00	8
	ATOM	1133	N	PRO			83.916	20.494	-2.582	1.00 20.00	7
45	ATOM	1134	CD	PRO			83.153	19.378	-1.993	1.00 20.00	6
	ATOM	1135	CA	PRO			85.122	20.005	-3.259	1.00 20.00	6
	ATOM	1136	CB	PRO			84.922	18.494	-3.267	1.00 20.00	6
	ATOM	1137	CG	PRO			84.174	18.256	-1.984	1.00 20.00	6
	ATOM	1138	C	PRO			85.303	20.574	-4.666	1.00 20.00	6
50	ATOM	1139	0	PRO			86.431	20.752	-5.124	1.00 20.00	8
50	ATOM	1140	N	GLU			84.197	20.752	-5.347	1.00 20.00	7
							84.243	21.410			6
	ATOM	1141	CA	GLU					-6.705	1.00 20.00	
	MOTA	1142	CB	GLU			82.836	21.424	-7.317	1.00 20.00	6
	MOTA	1143	CG	GLU			82.755	22.081	-8.690	1.00 20.00	6
55	MOTA	1144	CD	GLU			81.323	22.296	-9.159	1.00 20.00	6
	MOTA	1145	OE1	GLU			80.587	21.299	-9.322	1.00 20.00	8
	MOTA	1146	OE2	GLU			80.933	23.465	-9.364	1.00 20.00	8
	MOTA	1147	С	GLU			84.810	22.836	-6.716	1.00 20.00	6
	MOTA	1148	0	GLU	В	209	85.409	23.269	-7.705	1.00 20.00	8

	ATOM	1149	N	ASN	В	210	84.604	23.549	-5.612	1.00 20.0	0 7
	ATOM	1150	CA	ASN			85.051	24.932	-5.439	1.00 20.0	
	ATOM	1151	CB	ASN			84.033	25.695	-4.588	1.00 20.0	
	ATOM	1152	CG	ASN			82.851	26.170	-5.396	1.00 20.0	
5	ATOM	1153		ASN			81.807	26.520	-4.846	1.00 20.0	
-	ATOM	1154	ND2	ASN			83.010	26.194	-6.717	1.00 20.0	
	ATOM	1155	C	ASN			86,427	25.070	-4.797	1.00 20.0	
	ATOM	1156	Ö	ASN			86.937	26.181	-4.641	1.00 20.0	
	ATOM	1157		ILE			87.016	23.948	-4.406	1.00 20.0	
10			N								
10	ATOM	1158	CA			211	88.331	23.958	-3.790	1.00 20.0	
	ATOM	1159	CB	ILE			88.336	23.090	-2.521	1.00 20.0	
	ATOM	1160		ILE			89.732	23.025	-1.925	1.00 20.0	
	MOTA	1161		ILE			87.350	23.682	-1.510	1.00 20.0	
	MOTA	1162		ILE			87.121	22.832	-0.285	1.00 20.0	
15	MOTA	1163	C	ILE			89.307	23.414	-4.816	1.00 20.0	
	ATOM	1164	0			211	89.475	22.199	-4.949	1.00 20.0	
	MOTA	1165	N	LEU			89.938	24.319	-5.558	1.00 20.0	
	MOTA	1166	CA	LEU			90.875	23.918	-6.601	1.00 20.0	
	MOTA	1167	CB	LEU	В	212	90.966	25.012	-7.673	1.00 20.0	0 6
20	MOTA	1168	CG	LEU	В	212	89.630	25.510	-8.235	1.00 20.0	0 6
	MOTA	1169	CD1	LEU	В	212	89.896	26.462	-9.390	1.00 20.0	0 6
	MOTA	1170	CD2	LEU	В	212	88.781	24.331	-8.709	1.00 20.0	0 6
	ATOM	1171	С	LEU	В	212	92.254	23.628	-6.038	1.00 20.0	0 6
	ATOM	1172	0	LEU	В	212	92.537	23.923	-4.873	1.00 20.0	0 8
25	ATOM	1173	N	LEU	В	213	93.114	23.053	-6.875	1.00 20.0	0 7
	ATOM	1174	CA	LEU	В	213	94.472	22.714	-6.472	1.00 20.0	0 6
	ATOM	1175	CB	LEU	В	213	94.609	21.192	-6.388	1.00 20.0	0 6
	ATOM	1176	CG	LEU	В	213	93.775	20.526	-5.292	1.00 20.0	0 6
	ATOM	1177	CD1	LEU	В	213	93.737	19.035	-5.508	1.00 20.0	0 6
30	ATOM	1178	CD2	LEU	В	213	94.374	20.852	-3.935	1.00 20.0	0 6
	ATOM	1179	C	LEU			95.503	23.277	-7.449	1.00 20.0	
	ATOM	1180	ō	LEU			95.422	23.033	-8.657	1.00 20.0	
	ATOM	1181	N	ASN			96.470	24.036	-6.940	1.00 20.0	
	ATOM	1182	CA	ASN			97.488	24.585	-7.826	1.00 20.0	
35	ATOM	1183	CB	ASN			98.198	25.792	-7.201	1.00 20.0	
-	ATOM	1184	CG	ASN			98.938	25.448	-5.927	1.00 20.0	
	ATOM	1185		ASN			99,267	24.288	-5.669	1.00 20.0	
	ATOM	1186		ASN			99.224	26.469	-5.123	1.00 20.0	
	ATOM	1187	C	ASN			98.508	23.515	-8.182	1.00 20.0	
40	ATOM	1188	Ö	ASN			98.420	22.372	-7.725	1.00 20.0	
70	ATOM	1189	N	GLU			99.482	23.894	-8.996	1.00 20.0	
	ATOM	1190	CA	GLU			100.514	22.965	-9.430	1.00 20.0	
	ATOM	1191	CB	GLU			101.491	23.687	-10.362	1.00 20.0	
	ATOM	1192	CG	GLU			102.544	22.788	-10.362	1.00 20.0	
45	ATOM	1193	CD	GLU				23.482	-12.080	1.00 20.0	
43		1194					103.323	24.554			
	ATOM			GLU			103.909		-11.810	1.00 20.0	
	ATOM	1195 1196		GLU			103.344		-13.215	1.00 20.0	
	ATOM		C	GLU			101.275	22.307	-8.274	1.00 20.0	
50	MOTA	1197	0	GLU			101.801	21.205	-8.428	1.00 20.0	
30	MOTA	1198	N	ASP			101.335	22.976	-7.123	1.00 20.0	
	ATOM	1199	CA	ASP			102.036	22.430	-5.958	1.00 20.0	
	ATOM	1200	CB	ASP			102.727	23.549	-5.179	1.00 20.0	
	MOTA	1201	CG	ASP			103.952	24.086	-5.896	1.00 20.0	
	MOTA	1202		ASP			104.766	23.267	-6.376	1.00 20.0	
55	MOTA	1203		ASP			104.110	25.323	-5.973	1.00 20.0	
	MOTA	1204	C	ASP			101.121	21.651	-5.013	1.00 20.0	
	MOTA	1205	0	ASP	В		101.532	21.241	-3.925	1.00 20.0	
	MOTA	1206	N	MET			99.877	21.463	-5.434	1.00 20.0	
	ATOM	1207	CA	MET	В	217	98.890	20.730	-4.657	1.00 20.0	0 6

	MOTA	1208	CB	MET			99.402	19.319	-4.358		20.00	6
	MOTA	1209	CG			217	99.456	18.432	-5.601		20.00	6
	ATOM	1210	SD	MET			97.857	18.342	-6.445		20.00	16
	ATOM	1211	CE	MET		217	97.073	16.984	-5.543		20.00	6
5	ATOM	1212	C	MET			98.397	21.403	-3.373		20.00	6
	MOTA	1213	0	MET	В	217	97.972	20.730	-2.435	1.00	20.00	8
	MOTA	1214	N	HIS	В	218	98.469	22.730	-3.331	1.00	20.00	7
	ATOM	1215	CA	HIS	В	218	97.949	23.487	-2.197	1.00	20.00	6
	ATOM	1216	CB	HIS	В	218	98.831	24.700	-1.898	1.00	20.00	6
10	ATOM	1217	CG	HIS	В	218	100.100	24.357	-1.177	1.00	20.00	6
	MOTA	1218	CD2	HIS	В	218	101.390	24.362	-1.588	1.00	20.00	6
	ATOM	1219	ND1	HIS	В	218	100.117	23.935	0.136	1.00	20.00	7
	ATOM	1220	CE1	HIS	В	218	101.364	23.698	0.504	1.00	20.00	6
	ATOM	1221	NE2	HIS	В	218	102.156	23.947	-0.524	1.00	20.00	7
15	ATOM	1222	С	HIS	В	218	96.583	23.939	-2.703	1.00	20.00	6
	ATOM	1223	0	HIS	В	218	96.400	24.090	-3.910	1.00	20.00	8
	ATOM	1224	N	ILE	В	219	95.628	24.160	-1.808	1.00	20.00	7
	ATOM	1225	CA	ILE		219	94.301	24.562	-2.257		20.00	6
	ATOM	1226	CB	ILE		219	93.232	24.359	-1.159		20.00	6
20	ATOM	1227	CG2			219	93.266	22.918	-0.654		20.00	6
	ATOM	1228	CG1				93.460	25.353	-0.011		20.00	6
	ATOM	1229	CD1	ILE	В	219	92.351	25.342	1.036	1.00	20.00	6
	ATOM	1230	С	ILE	В	219	94.207	26.010	-2.714	1.00	20.00	6
	ATOM	1231	o			219	95.044	26.850	-2.375		20.00	8
25	ATOM	1232	N			220	93.168	26.274	-3.497		20.00	7
	ATOM	1233	CA	GLN			92.859	27.600	-3.999		20.00	6
	MOTA	1234	СВ			220	93.537	27.867	-5.350		20.00	6
	ATOM	1235	CG	GLN	В	220	95.011	28.246	-5.216	1.00	20.00	6
	ATOM	1236	CD	GLN	В	220	95.599	28.799	-6.503		20.00	6
30	ATOM	1237		GLN		220	95.725	28.086	-7.502		20.00	8
	ATOM	1238	NE2	GLN			95.957	30.079	-6.486		20.00	7
	ATOM	1239	С			220	91.350	27.626	-4.140		20.00	6
	ATOM	1240	ō			220	90.792	27.133	-5.124		20.00	8
	ATOM	1241	N			221	90.689	28.178	-3.129		20.00	7
35	ATOM	1242	CA			221	89.240	28.260	-3.122		20.00	6
	ATOM	1243	CB			221	88.731	28.550	-1.700		20.00	6
	ATOM	1244		ILE			87.209	28.707	-1.708		20.00	6
	ATOM	1245		ILE			89.164	27.406	-0.773		20.00	6
	ATOM	1246		ILE			88.743	27.559	0.668		20.00	6
40	ATOM	1247	С			221	88.760	29.339	-4.092		20.00	6
	ATOM	1248	ō			221	89.411	30.374	-4.262		20.00	8
	ATOM	1249	N			222	87.633	29.082	-4.748		20.00	7
	ATOM	1250	CA			222	87.084	30.039	-5.701		20.00	6
	ATOM	1251	CB			222	87.565	29.728	-7.125		20.00	6
45	ATOM	1252		THR			87.179	30.795	-8.000		20.00	8
	ATOM	1253	CG2	THR			86.962	28.410	-7.618		20.00	6
	ATOM	1254	C			222	85.554	30.028	-5.683		20.00	6
	ATOM	1255	ō			222	84.950	29.417	-4.791		20.00	8
	ATOM	1256	N	ASP			84.949	30.712	-6.659		20.00	7
50	ATOM	1257	CA	ASP			83.492	30.806	-6.806		20.00	6
50	ATOM	1258	CB			223	82.872	29.399	-6.767		20.00	6
	ATOM	1259	CG	ASP			81.414	29.384	-7.205	1.00		6
	ATOM	1260				223	80.990	30.335	-7.900		20.00	8
	ATOM	1261		ASP		223	80.701	28.414	-6.866	1.00		8
55	ATOM	1262	C	ASP		223	82.878	31.694	-5.725		20.00	6
22	ATOM	1263	0	ASP		223	82.191	31.208	-4.820	1.00		8
	ATOM	1264	N	PHE		224	83.105	33.001	-5.848		20.00	7
	ATOM	1265	CA	PHE			82.632	33.970	-4.866		20.00	6
	ATOM	1266	CB			224	83.800	34.869	-4.451		20.00	6
	111011	22.00	CD		-	~~ ~	33.000	51.005		1.00		0

	MOTA	1267	CG	PHE	В	224	84.826	34.165	-3.612	1.00	20.00	6
	ATOM	1268	CD1	PHE	В	224	84.590	33.931	-2.261	1.00	20.00	6
	MOTA	1269	CD2	PHE	В	224	86.001	33.687	-4.182	1.00	20.00	6
	MOTA	1270	CE1	PHE			85.509	33.227	-1.486		20.00	6
5	ATOM	1271	CE2				86.927	32.981	-3.418		20.00	6
-	ATOM	1272	CZ	PHE			86.679	32.750	-2.068		20.00	6
	ATOM	1273	C	PHE			81.443	34.839	-5.256		20.00	6
	ATOM	1274	o	PHE			81.001	35.678	-4.468		20.00	8
10	MOTA	1275	N	GLY			80.928	34.647	-6.463		20.00	7
10	ATOM	1276	CA	GLY			79.793	35.438	-6.894		20.00	6
	MOTA	1277	C	GLY			78.612	35.265	-5.955		20.00	6
	MOTA	1278	0	GLY			77.824	36.192	-5.753		20.00	8
	MOTA	1279	N	THR			78.486	34.080	-5.367		20.00	7
	ATOM	1280	CA	THR	В	226	77.379	33.819	-4.459	1.00	20.00	6
15	MOTA	1281	CB	THR	В	226	76.779	32.425	-4.715	1.00	20.00	6
	ATOM	1282	OG1	THR	В	226	77.826	31.450	-4.762	1.00	20.00	8
	MOTA	1283	CG2	THR	В	226	76.021	32.417	-6.041	1.00	20.00	6
	ATOM	1284	C	THR	В	226	77.738	33.957	-2.981	1.00	20.00	6
	ATOM	1285	0	THR	В	226	77.001	33.500	-2.107	1.00	20.00	8
20	ATOM	1286	N	ALA	В	227	78.867	34.598	-2.702	1.00	20.00	7
	ATOM	1287	CA	ALA			79.282	34.800	-1.325		20.00	6
	ATOM	1288	CB	ALA			80.738	35.242	-1.268		20.00	6
	ATOM	1289	C	ALA			78.384	35.875	-0.726		20.00	6
	ATOM	1290	ō	ALA			77.623	36.529	-1.440		20.00	8
25	ATOM	1291	N	LYS			78.467	36.046	0.586		20.00	7
23	ATOM	1292	CA	LYS			77.670	37.051	1.274		20.00	6
								36.384			20.00	
	ATOM	1293	CB	LYS			76.637		2.179			6
	MOTA	1294	CG	LYS			75.705	37.357	2.890		20.00	6
	MOTA	1295	CD	LYS			74.795	38.072	1.893		20.00	6
30	MOTA	1296	CE	LYS			73.849	39.049	2.587		20.00	6
	MOTA	1297	NZ	LYS			73.000	39.781	1.605		20.00	7
	MOTA	1298	C	LYS			78.616	37.896	2.110		20.00	6
	ATOM	1299	0	LYS			79.355	37.366	2.940		20.00	8
	ATOM	1300	N	VAL			78.603	39.206	1.881	1.00	20.00	7
35	MOTA	1301	CA	VAL			79.463	40.114	2.626	1.00	20.00	6
	ATOM	1302	CB	VAL	В	229	79.976	41.256	1.734	1.00	20.00	6
	ATOM	1303	CG1	VAL	В	229	80.853	42.191	2.540	1.00	20.00	6
	ATOM	1304	CG2	VAL	В	229	80.746	40.686	0.561	1.00	20.00	6
	ATOM	1305	С	VAL	В	229	78.687	40.710	3.793	1.00	20.00	6
40	ATOM	1306	0	VAL	В	229	77.798	41.537	3.599	1.00	20.00	8
	ATOM	1307	N	LEU	В	230	79.034	40.284	5.003	1.00	20.00	7
	ATOM	1308	CA	LEU			78.370	40.752	6.213		20.00	6
	ATOM	1309	CB	LEU			78.740	39.856	7.395		20.00	6
	ATOM	1310	CG	LEU			78.276	38.403	7.332		20.00	6
45	ATOM	1311		LEU			78.853	37.634	8.508		20.00	6
75	ATOM	1312		LEU			76.760	38.350	7.339		20.00	6
	ATOM	1313	C	LEU			78.705	42.193	6.565		20.00	6
	ATOM	1313	o	LEU			79.768	42.701	6.214		20.00	8
		1314	N	SER			77.781	42.701	7.270		20.00	7
50	MOTA											
30	MOTA	1316	CA	SER			77.957	44.219	7.708		20.00	6
	MOTA	1317	СВ	SER			77.082	45.161	6.875		20.00	6
	MOTA	1318	OG	SER			75.714	44.795	6.948		20.00	8
	MOTA	1319	C	SER			77.623	44.373	9.196		20.00	6
	MOTA	1320	0	SER			78.322	45.086	9.919		20.00	8
55	MOTA	1321	N	PRO			76.553	43.705	9.674		20.00	7
	MOTA	1322	CD	PRO			75.571	42.876	8.948		20.00	6
	MOTA	1323	CA	PRO		232	76.182	43.811	11.091		20.00	6
	MOTA	1324	CB	PRO	В	232	75.005	42.844	11.211	1.00	20.00	6
	ATOM	1325	CG	PRO	В	232	74.367	42.933	9.862	1.00	20.00	6

	ATOM	1326	C			232	77.332	43.438	12.024	1.00	20.00	6
	MOTA	1327	0	PRO	В	232	78.199	42.640	11.666	1.00	20.00	8
	MOTA	1328	N	ALA	В	237	74.215	38.132	11.762	1.00	20.00	7
	MOTA	1329	CA	ALA	В	237	74.666	37.653	10.460	1.00	20.00	6
5	ATOM	1330	CB	ALA	В	237	75.541	36.417	10.637	1.00	20.00	6
	ATOM	1331	C			237	73,479	37.324	9.558		20.00	6
	ATOM	1332	ō	ALA			73.143	36.158	9.374		20.00	8
	ATOM	1333	N	ALA			72.841	38.347	8.996		20.00	7
	ATOM	1334	CA	ALA			71.693	38.130	8.117		20.00	6
10							70.973					
10	ATOM	1335	CB	ALA				39.450	7.853		20.00	6
	ATOM	1336	С			238	72.123	37.497	6.798		20.00	6
	MOTA	1337	0	ALA			73.315	37.404	6.500		20.00	8
	MOTA	1338	N			239	71.146	37.057	6.012		20.00	7
	ATOM	1339	CA	ALA	В	239	71.439	36.431	4.728	1.00	20.00	6
15	MOTA	1340	CB	ALA	В	239	72.152	35.123	4.952	1.00	20.00	6
	ATOM	1341	C	ALA	В	239	70.173	36.194	3.918	1.00	20.00	6
	MOTA	1342	0	ALA	В	239	69.329	37.079	3.825	1.00	20.00	8
	ATOM	1343	N	ASN	В	240	70.068	34.996	3.339	1.00	20.00	7
	MOTA	1344	CA	ASN		240	68.939	34.559	2.514		20.00	6
20	MOTA	1345	СВ	ASN		240	67.614	35.160	2.999		20.00	6
	ATOM	1346	CG	ASN			67.258	36.466	2.299		20.00	6
	ATOM	1347		ASN			67.119	36.519	1.068		20.00	8
	ATOM	1348		ASN			67.091	37.536	3.089		20.00	7
		1349	C C	ASN			69.153	34.937	1.053		20.00	6
25	ATOM											
25	ATOM	1350	0	ASN			70.007	35.767	0.749		20.00	8
	ATOM	1351	N	ALA			68.365	34.329	0.163		20.00	7
	MOTA	1352	CA	ALA			68.401	34.570	-1.290		20.00	6
	MOTA	1353	С	ALA			68.990	33.416	-2.103		20.00	6
	MOTA	1354	0	ALA			68.353	32.919	-3.030		20.00	8
30	ATOM	1355	CB	ALA		241	69.168	35.859	-1.629		20.00	6
	ATOM	1356	N	PHE		242	70.205	33.000	-1.762	1.00	20.00	7
	ATOM	1357	CA	PHE	В	242	70.875	31.918	-2.481	1.00	20.00	6
	MOTA	1358	CB	PHE	В	242	72.259	32.379	-2.952	1.00	20.00	6
	ATOM	1359	CG	PHE	В	242	73.102	31.273	-3.521	1.00	20.00	6
35	ATOM	1360	CD1	PHE	В	242	72.843	30.767	-4.790		20.00	6
	ATOM	1361	CD2	PHE			74.136	30.713	-2.773		20.00	6
	ATOM	1362		PHE			73,599	29.718	-5.310		20.00	6
	ATOM	1363	CE2				74.896	29.666	-3.281		20.00	6
	ATOM	1364	CZ			242	74.627	29.166	-4.553		20.00	6
40	ATOM	1365	c			242	71.038	30.652	-1.646		20.00	6
40	ATOM	1366	o			242	71.038	30.632	-0.431		20.00	8
	ATOM	1367	N			243	70.988	29.505	-2.318		20.00	7
	ATOM	1368	CA	VAL			71.157	28.204	-1.675		20.00	6
	MOTA	1369	CB	VAL			69.828	27.420	-1.617		20.00	6
45	MOTA	1370		VAL			70.066	26.023	-1.050		20.00	6
	MOTA	1371	CG2				68.825	28.177	-0.766		20.00	6
	MOTA	1372	C	VAL	В	243	72.164	27.394	-2.486	1.00	20.00	6
	ATOM	1373	0	VAL	В	243	71.894	27.014	-3.628	1.00	20.00	8
	ATOM	1374	N	GLY	В	244	73.323	27.137	-1.890	1.00	20.00	7
50	ATOM	1375	CA	GLY			74.364	26.385	-2.569	1.00	20.00	6
	MOTA	1376	C			244	74.019	24.944	-2.911		20.00	6
	ATOM	1377	o			244	72.867	24.524	-2.810		20.00	8
	ATOM	1378	N			245	75.032	24.184	-3.315		20.00	7
	ATOM	1379	CA	THR			74.858	22.787	-3.691		20.00	6
55	MOTA	1379	CB			245	76.214	22.767	-4.046		20.00	6
,,												
	MOTA	1381		THR			76.794	22.911	-5.120		20.00	8
	ATOM	1382	CG2			245	76.049	20.710	-4.485		20.00	6
	MOTA	1383	С			245	74.174	22.003	-2.579		20.00	6
	MOTA	1384	0	THR	В	245	74.643	21.969	-1.441	1.00	20.00	8

	MOTA	1385	N	ALA			73.061	21.372	-2.937		20.00	7
	MOTA	1386	CA	ALA	В	246	72.229	20.615	-2.008	1.00	20.00	6
	MOTA	1387	CB	ALA	В	246	71.266	19.723	-2.793	1.00	20.00	6
	MOTA	1388	C	ALA	В	246	72.936	19.789	-0.941	1.00	20.00	6
5	ATOM	1389	0	ALA	В	246	72.611	19.894	0.239	1.00	20.00	8
	MOTA	1390	N	GLN	В	247	73.902	18.973	-1.339	1.00	20.00	7
	ATOM	1391	CA	GLN	В	247	74.580	18.121	-0.371	1.00	20.00	6
	ATOM	1392	CB	GLN	В	247	75.535	17.168	-1.096	1.00	20.00	6
	ATOM	1393	CG	GLN	В	247	75.110	16.823	-2.520	1.00	20.00	6
10	ATOM	1394	CD	GLN	В	247	75.139	15.336	-2.811	1.00	20.00	6
	ATOM	1395	OE1	GLN	В	247	75.963	14.602	-2.270	1.00	20.00	8
	ATOM	1396	NE2	GLN		247	74.246	14.887	-3.686		20.00	7
	ATOM	1397	С	GLN	В	247	75.343	18.873	0.720	1.00	20.00	6
	ATOM	1398	0	GLN	В	247	75.631	18.306	1.773	1.00	20.00	8
15	ATOM	1399	N	TYR	В	248	75.648	20.147	0.484	1.00	20.00	7
	ATOM	1400	CA	TYR	В	248	76.405	20.941	1.454	1.00	20.00	6
	ATOM	1401	CB	TYR	В	248	77.642	21.531	0.767	1.00	20.00	6
	ATOM	1402	CG	TYR		248	78.447	20.471	0.052		20.00	6
	ATOM	1403		TYR		248	79.329	19.648	0.750		20.00	6
20	ATOM	1404	CE1	TYR	В	248	79.979	18.589	0.115	1.00	20.00	6
	ATOM	1405	CD2	TYR	В	248	78.243	20.220	-1.306	1.00	20.00	6
	ATOM	1406	CE2	TYR	В	248	78.884	19.167	-1.951	1.00	20.00	6
	ATOM	1407	CZ	TYR	В	248	79.748	18.352	-1.232	1.00	20.00	6
	ATOM	1408	OH	TYR	В	248	80.348	17.280	-1.852	1.00	20.00	8
25	ATOM	1409	C	TYR	В	248	75.596	22.055	2.118	1.00	20.00	6
	ATOM	1410	0	TYR	В	248	76.132	22.824	2.917	1.00	20.00	8
	MOTA	1411	N	VAL	В	249	74.309	22.135	1.798	1.00	20.00	7
	MOTA	1412	CA	VAL	В	249	73.452	23.162	2.376	1.00	20.00	6
	MOTA	1413	CB	VAL	В	249	72.071	23.174	1.695	1.00	20.00	6
30	MOTA	1414	CG1	VAL	В	249	71.117	24.100	2.442	1.00	20.00	6
	ATOM	1415	CG2	VAL	В	249	72.225	23.632	0.264	1.00	20.00	6
	MOTA	1416	С	VAL	В	249	73.262	22.964	3.875	1.00	20.00	6
	MOTA	1417	0	VAL	В	249	73.027	21.847	4.341	1.00	20.00	8
	MOTA	1418	N	SER	В	250	73.373	24.055	4.628	1.00	20.00	7
35	ATOM	1419	CA	SER	В	250	73.206	24.008	6.076	1.00	20.00	6
	ATOM	1420	CB	SER	В	250	73.921	25.198	6.738	1.00	20.00	6
	MOTA	1421	OG	SER	В	250	73.428	26.440	6.257	1.00	20.00	8
	MOTA	1422	C	SER	В	250	71.717	24.049	6.405	1.00	20.00	6
	MOTA	1423	0	SER	В	250	70.920	24.577	5.636	1.00	20.00	8
40	MOTA	1424	N	PRO	В	251	71.322	23.479	7.550	1.00	20.00	7
	ATOM	1425	CD	PRO	В	251	72.130	22.770	8.558	1.00	20.00	6
	MOTA	1426	CA	PRO	В	251	69.905	23.484	7.925	1.00	20.00	6
	MOTA	1427	CB	PRO	В	251	69.892	22.714	9.252	1.00	20.00	6
	MOTA	1428	CG	PRO	В	251	71.290	22.936	9.801	1.00	20.00	6
45	MOTA	1429	C	PRO	В		69.265	24.870	8.032	1.00	20.00	6
	MOTA	1430	0	PRO	В	251	68.093	25.036	7.688	1.00	20.00	8
	ATOM	1431	N	GLU	В	252	70.017	25.867	8.492	1.00	20.00	7
	MOTA	1432	CA	GLU	В	252	69.462	27.216	8.625	1.00	20.00	6
	MOTA	1433	CB	GLU	В	252	70.503	28.193	9.196	1.00	20.00	6
50	MOTA	1434	CG	GLU	В	252	71.838	28.180	8.477	1.00	20.00	6
	MOTA	1435	CD	GLU	В	252	72.844	27.257	9.139	1.00	20.00	6
	MOTA	1436	OE1	GLU	В	252	72.429	26.207	9.675	1.00	20.00	8
	MOTA	1437	OE2	GLU		252	74.053	27.581	9.118	1.00	20.00	8
	MOTA	1438	C	GLU		252	68.928	27.744	7.292	1.00	20.00	6
55	MOTA	1439	0	GLU		252	67.927	28.459	7.261		20.00	8
	MOTA	1440	N	LEU		253	69.584	27.395	6.189		20.00	7
	MOTA	1441	CA	LEU		253	69.117	27.850	4.883	1.00	20.00	6
	MOTA	1442	CB	LEU		253	70.140	27.527	3.794		20.00	6
	MOTA	1443	CG	LEU	В	253	71.127	28.635	3.421	1.00	20.00	6

	ATOM	1444	CD1	LEU	В	253	72.121	28.851	4.547	1.00	20.00	6
	ATOM	1445	CD2	LEU	В	253	71.858	28.250	2.140	1.00	20.00	6
	ATOM	1446	C	LEU	В	253	67.774	27.227	4.496	1.00	20.00	6
	ATOM	1447	ō			253	66.997	27.826	3.751		20.00	8
5	ATOM	1448	N	LEU			67.506	26.029	5.002		20.00	7
-	ATOM	1449	CA	LEU			66.271	25.316	4.689		20.00	6
	ATOM	1450	CB	LEU		254	66.539	23.809	4.689		20.00	6
	ATOM	1451	CG	LEU			67.647	23.322	3.746		20.00	6
	ATOM	1451		LEU			67.983	21.873	4.057		20.00	6
10												
10	ATOM	1453		LEU			67.204	23.475	2.302		20.00	6
	ATOM	1454	С	LEU		254	65.135	25.626	5.662		20.00	6
	MOTA	1455	0	LEU			63.959	25.524	5.312		20.00	8
	MOTA	1456	N	THR			65.483	26.010	6.883		20.00	7
	MOTA	1457	CA	THR		255	64.472	26.308	7.884		20.00	6
15	MOTA	1458	CB	THR		255	64.876	25.747	9.252		20.00	6
	ATOM	1459	OG1	THR	В	255	66.154	26.277	9.619	1.00	20.00	8
	MOTA	1460	CG2	THR	В	255	64.958	24.230	9.202	1.00	20.00	6
	ATOM	1461	C	THR	В	255	64.205	27.795	8.035	1.00	20.00	6
	ATOM	1462	0	THR	В	255	63.072	28.241	7.897	1.00	20.00	8
20	ATOM	1463	N	GLU	В	256	65.250	28.560	8.314	1.00	20.00	7
	ATOM	1464	CA	GLU	В	256	65.115	30.001	8.507	1.00	20.00	6
	ATOM	1465	CB	GLU	В	256	66.015	30.444	9.659	1.00	20.00	6
	ATOM	1466	CG			256	65.634	29.818	10.987		20.00	6
	ATOM	1467	CD			256	66.736	29.922	12.018		20.00	6
25	ATOM	1468		GLU			67.249	31.041	12.232		20.00	8
	ATOM	1469	OE2	GLU			67.086	28.884	12.619		20.00	8
	ATOM	1470	C	GLU		256	65.439	30.815	7.262		20.00	6
	ATOM	1471	Ö	GLU			65.268	32.034	7.252		20.00	8
	ATOM	1472	N	LYS		257	65.906	30.141	6.215		20.00	7
30	ATOM	1472	CA	LYS		257	66.260	30.814	4.970		20.00	6
30	ATOM	1474	CB	LYS		257	65.015	31.458	4.352		20.00	6
			CG					31.438	2.915		20.00	
	ATOM	1475		LYS			65.184					6
	ATOM	1476	CD	LYS			63.885	32.497	2.378		20.00	6
	ATOM	1477	CE	LYS			63.994	32.841	0.902		20.00	6
35	ATOM	1478	NZ	LYS			65.060	33.847	0.640		20.00	7
	ATOM	1479	C	LYS			67.309	31.885	5.263		20.00	6
	MOTA	1480	0	LYS			67.270	32.977	4.702		20.00	8
	MOTA	1481	N			258	68.243	31.563	6.152		20.00	7
	MOTA	1482	CA			258	69.300	32.494	6.527		20.00	6
40	MOTA	1483	CB			258	69.043	33.028	7.937		20.00	6
	ATOM	1484	OG			258	68.893	31.962	8.859		20.00	8
	MOTA	1485	С	SER	В	258	70.675	31.829	6.467	1.00	20.00	6
	ATOM	1486	0	SER	В	258	70.786	30.602	6.542	1.00	20.00	8
	ATOM	1487	N	ALA	В	259	71.718	32.641	6.329	1.00	20.00	7
45	ATOM	1488	CA	ALA	В	259	73.081	32.130	6.252	1.00	20.00	6
	MOTA	1489	CB	ALA	В	259	73.549	32.121	4.809	1.00	20.00	6
	ATOM	1490	C	ALA	В	259	74.031	32.966	7.102	1.00	20.00	6
	ATOM	1491	0	ALA			73.882	34.185	7.211		20.00	8
	MOTA	1492	N	CYS			75.008	32.298	7.704		20.00	7
50	ATOM	1493	CA	CYS			75.993	32.960	8.550		20.00	6
	ATOM	1494	СВ	CYS			75.574	32.865	10.017		20.00	6
	ATOM	1495	SG			260	75.303	31.165	10.594		20.00	
	ATOM	1496	c	CYS		260	77.328	32.265	8.349		20.00	6
	ATOM	1497	0	CYS		260	77.410	31.280	7.620		20.00	8
55	ATOM	1498	N	LYS			78.371	32.775	8.993		20.00	7
23	ATOM	1499	CA	LYS			79.691	32.174	8.869		20.00	6
		1500	CB	LYS		261					20.00	
	MOTA	1500	CG				80.676 80.985	32.851	9.821			6
	ATOM					261		34.296	9.472		20.00	6
	MOTA	1502	CD	LYS	В	261	81.961	34.878	10.475	1.00	20.00	6

	ATOM	1503	CE	LYS	В	261	82.157	36.365	10.259	1.00 20.00	6
	ATOM	1504	NZ			261	83.085	36.922	11.278	1.00 20.00	7
	ATOM	1505	C	LYS		261	79.632	30.687	9.187	1.00 20.00	6
	ATOM	1506	ō	LYS		261	80.258	29.877	8.512	1.00 20.00	8
5	ATOM	1507	N			262	78.860	30.346	10.214	1.00 20.00	7
5	ATOM	1508	CA			262	78.716	28.966	10.659	1.00 20.00	6
	MOTA	1509	CB	SER		262	77.806	28.913	11.895	1.00 20.00	6
	MOTA	1510	OG			262	77.884	27.657	12.546	1.00 20.00	8
	MOTA	1511	C			262	78.161	28.070	9.549	1.00 20.00	6
10	MOTA	1512	0			262	78.350	26.856	9.575	1.00 20.00	8
	MOTA	1513	N	SER		263	77.466	28.660	8.581	1.00 20.00	7
	MOTA	1514	CA	SER	В	263	76.938	27.870	7.472	1.00 20.00	6
	MOTA	1515	CB	SER	В	263	76.132	28.750	6.507	1.00 20.00	6
	ATOM	1516	OG	SER	В	263	75.011	29.329	7.156	1.00 20.00	8
15	MOTA	1517	C	SER	В	263	78.123	27.244	6.737	1.00 20.00	6
	ATOM	1518	0	SER	В	263	78.038	26.108	6.273	1.00 20.00	8
	ATOM	1519	N	ASP	В	264	79.234	27.977	6.642	1.00 20.00	7
	ATOM	1520	CA	ASP	В	264	80.419	27.448	5.961	1.00 20.00	6
	ATOM	1521	CB	ASP		264	81.478	28.538	5.745	1.00 20.00	6
20	ATOM	1522	CG	ASP		264	81.091	29.539	4.673	1.00 20.00	6
20	ATOM	1523		ASP		264	80.286	29.187	3.786	1.00 20.00	8
	ATOM	1524		ASP			81.617	30.676	4.704	1.00 20.00	8
	ATOM	1525		ASP			81.043	26.312		1.00 20.00	6
			C						6.771		
2.5	MOTA	1526	0	ASP			81.586	25.365	6.201	1.00 20.00	8
25	ATOM	1527	N			265	80.971	26.415	8.099	1.00 20.00	7
	MOTA	1528	CA	LEU		265	81.532	25.390	8.974	1.00 20.00	6
	MOTA	1529	CB	LEU		265	81.491	25.848	10.438	1.00 20.00	6
	MOTA	1530	CG	LEU			82.419	27.035	10.746	1.00 20.00	6
	MOTA	1531		LEU		265	82.204	27.532	12.177	1.00 20.00	6
30	MOTA	1532		LEU		265	83.864	26.608	10.541	1.00 20.00	6
	MOTA	1533	C	LEU		265	80.750	24.094	8.800	1.00 20.00	6
	ATOM	1534	0	LEU	В	265	81.306	23.004	8.910	1.00 20.00	8
	MOTA	1535	N	TRP	В	266	79.454	24.208	8.530	1.00 20.00	7
	MOTA	1536	CA	TRP	В	266	78.646	23.017	8.309	1.00 20.00	6
35	ATOM	1537	CB	TRP	В	266	77.167	23.384	8.148	1.00 20.00	6
	ATOM	1538	CG	TRP		266	76.310	22.245	7.646	1.00 20.00	6
	MOTA	1539		TRP			75.455	21.399	8.426	1.00 20.00	6
	ATOM	1540	CE2			266	74.881	20.455	7.542	1.00 20.00	6
	ATOM	1541		TRP			75.117	21.345	9.785	1.00 20.00	6
40	ATOM	1542		TRP		266	76.220	21.792	6.356	1.00 20.00	6
70	ATOM	1543		TRP		266	75.365	20.719	6.288	1.00 20.00	7
	ATOM	1544	CZ2	TRP		266	73.988	19.466	7.975	1.00 20.00	6
	ATOM	1545		TRP		266	74.227	20.359	10.216	1.00 20.00	6
4.5	MOTA	1546		TRP		266	73.674	19.434	9.310	1.00 20.00	6
45	MOTA	1547	C	TRP		266	79.169	22.356	7.038	1.00 20.00	6
	MOTA	1548	0	TRP		266	79.356	21.142	6.988	1.00 20.00	8
	MOTA	1549	N	ALA		267	79.411	23.164	6.011	1.00 20.00	7
	MOTA	1550	CA	ALA			79.930	22.646	4.751	1.00 20.00	6
	MOTA	1551	CB	ALA			80.089	23.772	3.746	1.00 20.00	6
50	MOTA	1552	C	ALA	В	267	81.277	21.976	5.016	1.00 20.00	6
	MOTA	1553	0	ALA	В	267	81.570	20.914	4.471	1.00 20.00	8
	MOTA	1554	N	LEU	В	268	82.091	22.596	5.864	1.00 20.00	7
	ATOM	1555	CA	LEU		268	83.393	22.030	6.209	1.00 20.00	6
	ATOM	1556	CB	LEU		268	84.092	22.898	7.264	1.00 20.00	6
55	MOTA	1557	CG	LEU		268	85.379	22.332	7.879	1.00 20.00	6
	ATOM	1558		LEU			86.442	22.192	6.803	1.00 20.00	6
	ATOM	1559		LEU		268	85.872	23.263	9.006	1.00 20.00	6
	ATOM	1560	C			268	83.193	20.617	6.753	1.00 20.00	6
	ATOM	1561	0			268	83.903	19.684	6.372	1.00 20.00	8
	MIUM	TOPT	-	Tre C	ń	200	03.903	10.684	0.3/2	1.00 20.00	- 8

	MOTA	1562	N	GLY	В	269	82.220	20.463	7.645	1.00 20.00	7
	ATOM	1563	CA			269	81.947	19.156	8.217	1.00 20.00	6
	ATOM	1564	С	GLY		269	81.597	18.125	7.156	1.00 20.00	6
	ATOM	1565	ō			269	82.025	16.971	7.239	1.00 20.00	8
5	ATOM	1566	N			270	80.819	18.530	6.155	1.00 20.00	7
-	ATOM	1567	CA			270	80.445	17.613	5.083	1.00 20.00	6
	ATOM	1568	CB	CYS		270	79.413	18.255	4.148	1.00 20.00	6
	ATOM	1569	SG			270	77.824	18.654	4.905		
10	MOTA	1570	С			270	81.682	17.241	4.265	1.00 20.00	6
10	MOTA	1571	0			270	81.852	16.090	3.866	1.00 20.00	8
	MOTA	1572	N			271	82.541	18.226	4.012	1.00 20.00	7
	ATOM	1573	CA			271	83.751	18.000	3.229	1.00 20.00	6
	MOTA	1574	CB			271	84.436	19.339	2.903	1.00 20.00	6
	MOTA	1575	CG2	ILE	В	271	85.784	19.098	2.227	1.00 20.00	6
15	MOTA	1576	CG1	ILE	В	271	83.508	20.171	2.007	1.00 20.00	6
	ATOM	1577	CD1	ILE	В	271	83.962	21.607	1.815	1.00 20.00	6
	MOTA	1578	C	ILE	В	271	84.729	17.063	3.934	1.00 20.00	6
	ATOM	1579	0	ILE	В	271	85.300	16.174	3.304	1.00 20.00	8
	MOTA	1580	N	ILE	В	272	84.927	17.258	5.236	1.00 20.00	7
20	ATOM	1581	CA			272	85.820	16.382	5.987	1.00 20.00	6
	ATOM	1582	СВ			272	85.902	16.790	7.471	1.00 20.00	6
	ATOM	1583		ILE			86.623	15.703	8.277	1.00 20.00	6
	ATOM	1584		ILE			86.646	18.120	7.606	1.00 20.00	6
	ATOM	1585		ILE			86.553	18.723	9.011	1.00 20.00	6
25	ATOM	1586	C			272	85.274	14.957	5.901	1.00 20.00	6
23	ATOM	1587	Ö			272	86.021	14.003	5.679	1.00 20.00	8
											7
	ATOM	1588	N			273	83.964	14.822	6.072	1.00 20.00	
	ATOM	1589	CA			273	83.324	13.518	6.006	1.00 20.00	6
	MOTA	1590	CB			273	81.825	13.651	6.287	1.00 20.00	6
30	MOTA	1591	CG			273	81.064	12.340	6.250	1.00 20.00	6
	MOTA	1592		TYR			80.806	11.690	5.041	1.00 20.00	6
	ATOM	1593		TYR			80.107	10.486	5.005	1.00 20.00	6
	MOTA	1594		TYR			80.601	11.750	7.427	1.00 20.00	6
	ATOM	1595	CE2	TYR			79.904	10.548	7.405	1.00 20.00	6
35	MOTA	1596	CZ			273	79.659	9.922	6.192	1.00 20.00	6
	ATOM	1597	OH	TYR	В	273	78.971	8.736	6.174	1.00 20.00	8
	MOTA	1598	C	TYR	В	273	83.550	12.897	4.632	1.00 20.00	6
	MOTA	1599	0	TYR	В	273	83.865	11.713	4.526	1.00 20.00	8
	MOTA	1600	N	GLN	В	274	83.402	13.705	3.586	1.00 20.00	7
40	MOTA	1601	CA	GLN	В	274	83.579	13.230	2.220	1.00 20.00	6
	ATOM	1602	CB	GLN	В	274	83.176	14.322	1.222	1.00 20.00	6
	ATOM	1603	CG	GLN	В	274	83.149	13.857	-0.230	1.00 20.00	6
	ATOM	1604	CD	GLN		274	82.558	14.898	-1.169	1.00 20.00	6
	ATOM	1605		GLN			82.108	15.961	-0.736	1.00 20.00	8
45	MOTA	1606		GLN			82.548	14.591	-2.462	1.00 20.00	7
	ATOM	1607	C	GLN			85.013	12.788	1.953	1.00 20.00	6
	ATOM	1608	ō	GLN			85.239	11.818	1.233	1.00 20.00	8
	ATOM	1609	N			275	85.981	13.498	2.528	1.00 20.00	7
	ATOM	1610	CA	LEU			87.389	13.143	2.333	1.00 20.00	6
50			CB	LEU			88.311	14.194	2.971	1.00 20.00	
30	ATOM	1611									6
	ATOM	1612	CG			275	88.418	15.561	2.284	1.00 20.00	6
	ATOM	1613		LEU			89.325	16.481	3.088	1.00 20.00	6
	MOTA	1614		LEU			88.969	15.379	0.879	1.00 20.00	6
	MOTA	1615	C			275	87.697	11.779	2.940	1.00 20.00	6
55	MOTA	1616	0			275	88.430	10.981	2.354	1.00 20.00	8
	MOTA	1617	N			276	87.125	11.519	4.112	1.00 20.00	7
	MOTA	1618	CA	VAL		276	87.353	10.269	4.827	1.00 20.00	6
	MOTA	1619	CB	VAL			87.096	10.451	6.342	1.00 20.00	6
	ATOM	1620	CG1	VAL	В	276	87.376	9.148	7.082	1.00 20.00	6

	ATOM	1621	CG2	VAL	В	276	87.973	11.580	6.891	1.00	20.00	6
	ATOM	1622	C	VAL	В	276	86.504	9.089	4.336	1.00	20.00	6
	ATOM	1623	0	VAL	В	276	87.005	7.973	4.195	1.00	20.00	8
	ATOM	1624	N	ALA	В	277	85.222	9.337	4.090	1.00	20.00	7
5	ATOM	1625	CA	ALA			84.310	8.291	3.643		20.00	6
	ATOM	1626	CB	ALA			82.898	8.597	4.124		20.00	6
	ATOM	1627	C	ALA		277	84.315	8.115	2.130		20.00	6
	ATOM	1628	o	ALA			84.036	7.029	1.627		20.00	8
	ATOM	1629	N	GLY			84.632	9.180	1.405		20.00	7
10	ATOM	1630	CA	GLY			84.653	9.099	-0.041		20.00	6
10	ATOM	1631	C	GLY			83.365	9.627	-0.644		20.00	6
												8
	ATOM	1632	0	GLY			83.272	9.817	-1.860		20.00	7
	ATOM	1633	N	LEU			82.375	9.867	0.211		20.00	
	ATOM	1634	CA	LEU			81.075	10.382	-0.219		20.00	6
15	ATOM	1635	CB	LEU		279	80.070	9.232	-0.375		20.00	6
	ATOM	1636	CG	LEU			80.342	8.114	-1.385		20.00	6
	ATOM	1637		LEU		279	79.311	7.009	-1.191		20.00	6
	MOTA	1638		LEU		279	80.291	8.660	-2.804		20.00	6
	MOTA	1639	C	LEU		279	80.522	11.369	0.812		20.00	6
20	MOTA	1640	0	LEU		279	80.750	11.218	2.007		20.00	8
	MOTA	1641	N	PRO			79.787	12.395	0.361		20.00	7
	MOTA	1642	CD	PRO	В	280	79.403	12.730	-1.020	1.00	20.00	6
	ATOM	1643	CA	PRO	В	280	79.230	13.361	1.314	1.00	20.00	6
	ATOM	1644	CB	PRO	В	280	78.569	14.397	0.407	1.00	20.00	6
25	ATOM	1645	CG	PRO	В	280	78.191	13.598	-0.802	1.00	20.00	6
	ATOM	1646	C	PRO	В	280	78.242	12.662	2.262	1.00	20.00	6
	MOTA	1647	0	PRO	В	280	77.666	11.633	1.913	1.00	20.00	8
	ATOM	1648	N	PRO	В	281	78.035	13.220	3.470	1.00	20.00	7
	ATOM	1649	CD	PRO	В	281	78.571	14.535	3.859	1.00	20.00	6
30	ATOM	1650	CA	PRO	В	281	77.145	12.701	4.520	1.00	20.00	6
	ATOM	1651	CB	PRO			77.262	13.746	5.634		20.00	6
	ATOM	1652	CG	PRO			78.546	14.450	5.344		20.00	6
	ATOM	1653	C	PRO			75.679	12.485	4.142		20.00	6
	ATOM	1654	o	PRO			75.094	11.441	4.442		20.00	8
35	ATOM	1655	N	PHE			75.088	13.487	3.504		20.00	7
-	ATOM	1656	CA	PHE			73.686	13.427	3.123		20.00	6
	ATOM	1657	CB	PHE			73.006	14.734	3.531		20.00	6
	ATOM	1658	CG	PHE			73.300	15.146	4.947		20.00	6
	ATOM	1659		PHE			72.624	14.560	6.013		20.00	6
40	ATOM	1660		PHE			74.295	16.085	5.218		20.00	6
40	ATOM	1661		PHE			72.934	14.902	7.331		20.00	6
	ATOM	1662		PHE			74.613	16.433	6.530		20.00	6
	ATOM	1663	CZ	PHE			73.930	15.840	7.591		20.00	6
45	ATOM	1664	C	PHE			73.527	13.191	1.628		20.00	6
43	ATOM	1665	0	PHE			73.797	14.079	0.819		20.00	8
	ATOM	1666	N	ARG			73.080	11.994	1.267		20.00	7
	ATOM	1667	CA	ARG			72.888	11.635	-0.134		20.00	6
	MOTA	1668	CB	ARG			73.931	10.598	-0.559		20.00	6
	ATOM	1669	CG	ARG			75.358	10.928	-0.151		20.00	6
50	MOTA	1670	CD	ARG			76.326	9.883	-0.687		20.00	6
	MOTA	1671	NE	ARG			76.054	8.555	-0.142		20.00	7
	MOTA	1672	CZ	ARG			76.404	8.159	1.077		20.00	6
	MOTA	1673		ARG			77.047	8.986	1.893		20.00	7
	MOTA	1674		ARG			76.108	6.933	1.484		20.00	7
55	MOTA	1675	C	ARG			71.493	11.046	-0.331		20.00	6
	MOTA	1676	0	ARG			70.957	10.391	0.563		20.00	8
	MOTA	1677	N	ALA		284	70.911	11.276	-1.502		20.00	7
	MOTA	1678	CA	ALA			69.579	10.755	-1.796		20.00	6
	ATOM	1679	CB	ALA	В	284	68.532	11.484	-0.961	1.00	20.00	6

	ATOM	1680	C	ALA	В	284	69.278	10.921	-3.273	1.00 20.	.00	6
	ATOM	1681	0	ALA		284	70.007	11.611	-3.984	1.00 20.	.00	8
	MOTA	1682	N	GLY	В	285	68.191	10.299	-3.722	1.00 20.	.00	7
	ATOM	1683	CA	GLY		285	67.807	10.360	-5.122	1.00 20.		6
5	ATOM	1684	C	GLY			67.561	11.737	-5.707	1.00 20.		6
-	MOTA	1685	ō			285	67.775	11.955	-6.899	1.00 20.		8
	ATOM	1686	N	ASN		286	67.089	12.673	-4.892	1.00 20.		7
	ATOM	1687	CA	ASN			66.835	14.018	-5.386	1.00 20.		6
	ATOM	1688	CB	ASN			65.403	14.137	-5.930	1.00 20.		6
10												
10	ATOM	1689	CG	ASN		286	64.342	13.825	-4.885	1.00 20.		6
	MOTA	1690		ASN		286	64.292	14.450	-3.826	1.00 20.		8
	MOTA	1691		ASN			63.477	12.861	-5.190	1.00 20.		7
	MOTA	1692	C	ASN			67.076	15.042	-4.291	1.00 20.		6
	MOTA	1693	0	ASN		286	67.368	14.682	-3.152	1.00 20.		8
15	MOTA	1694	N	GLU		287	66.955	16.317	-4.636	1.00 20.		7
	ATOM	1695	CA	GLU	В	287	67.185	17.377	-3.669	1.00 20.	.00	6
	MOTA	1696	CB	GLU	В	287	67.181	18.738	-4.365	1.00 20.	.00	6
	ATOM	1697	CG	GLU	В	287	68.537	19.095	-4.944	1.00 20.	.00	6
	ATOM	1698	CD	GLU	В	287	68.524	20.385	-5.735	1.00 20.	.00	6
20	MOTA	1699	OE1	GLU	В	287	67.911	21.371	-5.267	1.00 20.	.00	8
	ATOM	1700	OE2	GLU	В	287	69.144	20.410	-6.823	1.00 20.	.00	8
	ATOM	1701	C	GLU	В	287	66.225	17.394	-2.492	1.00 20.	.00	6
	ATOM	1702	0	GLU		287	66.658	17.554	-1.354	1.00 20.		8
	MOTA	1703	N	TYR		288	64.932	17.233	-2.753	1.00 20.		7
25	ATOM	1704	CA	TYR		288	63.955	17.239	-1.670	1.00 20.		6
	ATOM	1705	CB	TYR		288	62.553	16.899	-2.184	1.00 20.		6
	ATOM	1706	CG	TYR		288	61.530	16.780	-1.070	1.00 20.		6
	ATOM	1707		TYR			60.984	17.917	-0.470	1.00 20.		6
	ATOM	1708		TYR		288	60.090	17.814	0.600	1.00 20.		6
30	ATOM	1709	CD2	TYR		288	61.154	15.529	-0.573	1.00 20.		6
30	ATOM	1710	CE2	TYR		288	60.265	15.414	0.498	1.00 20.		6
			CZ					16.561		1.00 20.		
	ATOM	1711				288	59.740		1.078			6
	ATOM	1712	OH	TYR			58.884	16.454	2.149	1.00 20.		8
	ATOM	1713	С	TYR			64.337	16.238	-0.587	1.00 20.		6
35	MOTA	1714	0	TYR			64.254	16.545	0.598	1.00 20.		8
	ATOM	1715	N	LEU			64.750	15.041	-1.001	1.00 20.		7
	MOTA	1716	CA	LEU			65.137	13.989	-0.064	1.00 20.		6
	MOTA	1717	CB	LEU		289	65.283	12.649	-0.797	1.00 20.		6
	MOTA	1718	CG	LEU		289	63.984	11.985	-1.274	1.00 20.		6
40	MOTA	1719		LEU		289	64.314	10.802	-2.179	1.00 20.		6
	MOTA	1720		LEU		289	63.160	11.530	-0.068	1.00 20.		6
	ATOM	1721	C	LEU		289	66.431	14.310	0.685	1.00 20.		6
	MOTA	1722	0	LEU	В	289	66.604	13.914	1.840	1.00 20.	.00	8
	ATOM	1723	N	ILE	В	290	67.340	15.017	0.025	1.00 20.	.00	7
45	ATOM	1724	CA	ILE	В	290	68.597	15.390	0.658	1.00 20.	.00	6
	MOTA	1725	CB	ILE	В	290	69.583	15.985	-0.366	1.00 20.	.00	6
	ATOM	1726	CG2	ILE	В	290	70.778	16.609	0.359	1.00 20.	.00	6
	ATOM	1727	CG1	ILE	В	290	70.046	14.887	-1.330	1.00 20.	00	6
	MOTA	1728		ILE	В	290	70.844	15.398	-2.518	1.00 20.		6
50	ATOM	1729	С			290	68.307	16.424	1.743	1.00 20.		6
	ATOM	1730	ō			290	68.807	16.317	2.862	1.00 20.		8
	ATOM	1731	N			291	67.491	17.420	1.411	1.00 20.		7
	ATOM	1732	CA	PHE		291	67.143	18.462	2.372	1.00 20.		6
	ATOM	1733	CB	PHE		291	66.222	19.502	1.731	1.00 20.		6
55	ATOM	1734	CG	PHE		291	66.869	20.289	0.628	1.00 20.		6
23	ATOM	1735		PHE		291	68.255	20.209	0.568	1.00 20.		6
		1735	CD1	PHE		291				1.00 20.		
	MOTA						66.094	20.931	-0.332			6
	MOTA	1737		PHE			68.859	21.182	-0.435	1.00 20.		6
	MOTA	1738	CE2	PHE	В	Z91	66.690	21.697	-1.340	1.00 20.	.UU	6

	ATOM	1739	CZ	PHE	В	291	68.074	21.822	-1.390	1.00 20.00	6
	ATOM	1740	C	PHE	В	291	66,453	17.848	3.576	1.00 20.00	6
	MOTA	1741	o	PHE		291	66.664	18.262	4.718	1.00 20.00	8
	ATOM	1742	N	GLN		292	65.629	16.847	3.303	1.00 20.00	7
5	ATOM	1743	CA			292	64.887	16.154	4.341	1.00 20.00	6
	ATOM	1744	CB			292	64.006	15.090	3.687	1.00 20.00	6
	ATOM	1745	CG	GLN		292	62.953	14.486	4.572	1.00 20.00	6
	ATOM	1746	CD			292	61.895	13.750	3.763	1.00 20.00	6
	ATOM	1747		GLN			62.208	12.835	2.997	1.00 20.00	8
10											
10	ATOM	1748	NE2			292	60.637	14.155	3.924	1.00 20.00	7
	ATOM	1749	С	GLN		292	65.865	15.522	5.329	1.00 20.00	6
	MOTA	1750	0			292	65.689	15.630	6.540	1.00 20.00	8
	MOTA	1751	N	LYS		293	66.907	14.875	4.812	1.00 20.00	7
	MOTA	1752	CA	LYS		293	67.898	14.244	5.683	1.00 20.00	6
15	MOTA	1753	CB	LYS		293	68.850	13.372	4.865	1.00 20.00	6
	MOTA	1754	CG	LYS	В	293	68.197	12.135	4.278	1.00 20.00	6
	MOTA	1755	CD	LYS	В	293	69.217	11.260	3.554	1.00 20.00	6
	MOTA	1756	CE	LYS	В	293	68.575	9.972	3.051	1.00 20.00	6
	ATOM	1757	NZ	LYS	В	293	69.553	9.099	2.339	1.00 20.00	7
20	ATOM	1758	C	LYS	В	293	68.698	15.287	6.468	1.00 20.00	6
	ATOM	1759	0	LYS	В	293	69.044	15.074	7.634	1.00 20.00	8
	MOTA	1760	N	ILE	В	294	68.989	16.411	5.827	1.00 20.00	7
	ATOM	1761	CA	ILE		294	69.745	17.480	6.472	1.00 20.00	6
	ATOM	1762	CB	ILE		294	70.026	18.632	5.474	1.00 20.00	6
25	ATOM	1763	CG2			294	70.489	19.881	6.223	1.00 20.00	6
	ATOM	1764		ILE		294	71.070	18.178	4.443	1.00 20.00	6
	ATOM	1765		ILE		294	71.266	19.159	3.303	1.00 20.00	6
	ATOM	1766	C	ILE		294	69.035	18.045	7.712	1.00 20.00	6
	ATOM	1767	Ö	ILE		294	69.618	18.091	8.798	1.00 20.00	8
30	ATOM	1768	N	ILE		295	67.783	18.467	7.564	1.00 20.00	7
30	ATOM	1769	CA	ILE		295	67.068	19.037	8.707	1.00 20.00	6
	ATOM	1770	CB			295	65.710	19.647	8.300	1.00 20.00	6
	ATOM	1771		ILE			65.927	20.749	7.265	1.00 20.00	6
	MOTA	1772		ILE		295	64.784	18.559	7.762	1.00 20.00	6
35	ATOM	1773		ILE			63.356	19.037	7.558	1.00 20.00	6
	ATOM	1774	C			295	66.831	18.045	9.842	1.00 20.00	6
	MOTA	1775	0			295	66.540	18.447	10.967	1.00 20.00	8
	MOTA	1776	N	LYS		296	66.956	16.753	9.550	1.00 20.00	7
	MOTA	1777	CA			296	66.765	15.724	10.569	1.00 20.00	6
40	MOTA	1778	CB	LYS		296	65.907	14.576	10.019	1.00 20.00	6
	MOTA	1779	CG	LYS		296	64.535	15.010	9.538	1.00 20.00	6
	MOTA	1780	CD	LYS		296	63.739	13.851	8.951	1.00 20.00	
	MOTA	1781	CE	LYS	В	296	63.296	12.873	10.025	1.00 20.00	6
	MOTA	1782	NZ	LYS	В	296	62.375	11.828	9.482	1.00 20.00	7
45	ATOM	1783	C	LYS	В	296	68.116	15.176	11.018	1.00 20.00	6
	MOTA	1784	0	LYS	В	296	68.178	14.261	11.838	1.00 20.00	8
	MOTA	1785	N	LEU	В	297	69.190	15.746	10.474	1.00 20.00	7
	MOTA	1786	CA	LEU	В	297	70.551	15.320	10.791	1.00 20.00	6
	MOTA	1787	CB	LEU	В	297	70.911	15.680	12.236	1.00 20.00	6
50	ATOM	1788	CG	LEU		297	72.398	15.538	12.585	1.00 20.00	
	ATOM	1789		LEU			73.215	16.555	11.771	1.00 20.00	6
	ATOM	1790		LEU			72.605	15.762	14.076	1.00 20.00	6
	ATOM	1791	C	LEU		297	70.635	13.810	10.592	1.00 20.00	6
	ATOM	1792	Ö	LEU		297	71.150	13.080	11.434	1.00 20.00	
55	ATOM	1793	N	GLU			70.128	13.351	9.456	1.00 20.00	7
55	ATOM	1794	CA			298	70.128	11.934	9.148	1.00 20.00	6
	MOTA	1794	CB	GLU		298	68.817	11.597	8.416	1.00 20.00	6
	ATOM	1795	CG			298	68.817		8.416	1.00 20.00	6
								10.123			
	MOTA	1797	CD	التك	Ľ	298	67.254	9.858	7.535	1.00 20.00	6

	ATOM	1798	OE1	GLU	В	298	66.214	10.331	8.043	1.00 2	0.00	8
	ATOM	1799		GLU			67.261	9.185	6.484	1.00 2		8
	MOTA	1800	C	GLU		298	71.309	11.446	8.332	1.00 2		6
	ATOM	1801	ō	GLU		298	71.310	11.523	7.104	1.00 2		8
5	ATOM	1802	N	TYR		299	72.325	10.946	9.027	1.00 2		7
,	ATOM	1803	CA	TYR		299	73.519	10.405	8.390	1.00 2		6
	ATOM	1804	CB	TYR		299	74.444	11.521	7.880	1.00 2		6
	MOTA	1805	CG	TYR		299	75.330	12.130	8.953	1.00 2		6
	MOTA	1806		TYR		299	74.796	12.962	9.935	1.00 2		6
10	MOTA	1807		TYR		299	75.589	13.482	10.951	1.00 2		6
	MOTA	1808	CD2	TYR		299	76.692	11.833	9.013	1.00 2		6
	ATOM	1809	CE2	TYR	В	299	77.499	12.352	10.032	1.00 2	0.00	6
	MOTA	1810	CZ	TYR	В	299	76.935	13.173	10.995	1.00 2	0.00	6
	MOTA	1811	OH	TYR	В	299	77.701	13.687	12.006	1.00 2	0.00	8
15	ATOM	1812	C	TYR	В	299	74.245	9.600	9.456	1.00 2	0.00	6
	ATOM	1813	0	TYR	В	299	73.913	9.688	10.631	1.00 2	0.00	8
	ATOM	1814	N	ASP	В	300	75.229	8.808	9.052	1.00 2	0.00	7
	ATOM	1815	CA	ASP	В	300	75.991	8.030	10.016	1.00 2	0.00	6
	ATOM	1816	CB	ASP		300	75.291	6.700	10.304	1.00 2		6
20	ATOM	1817	CG		В	300	74.898	5.968	9.048	1.00 2		6
20	ATOM	1818		ASP		300	75.806	5.594	8.274	1.00 2		8
	ATOM	1819		ASP		300	73.681	5.771	8.832	1.00 2		8
	ATOM	1820	С	ASP		300	77.397	7.799	9.488	1.00 2		6
2.5	ATOM	1821	0	ASP		300	77.651	7.976	8.297	1.00 2		8
25	MOTA	1822	N	PHE		301	78.307	7.417	10.378	1.00 2		7
	MOTA	1823	CA	PHE		301	79.695	7.186	9.996	1.00 2		6
	MOTA	1824	CB	PHE		301	80.655	7.664	11.093	1.00 2		6
	MOTA	1825	CG	PHE		301	80.488	9.103	11.481	1.00 2		6
	ATOM	1826		PHE		301	79.493	9.487	12.370	1.00 2		6
30	MOTA	1827	CD2	PHE	В	301	81.346	10.075	10.970	1.00 2	0.00	6
	ATOM	1828	CE1	PHE	В	301	79.352	10.823	12.750	1.00 2	0.00	6
	MOTA	1829	CE2	PHE	В	301	81.214	11.408	11.342	1.00 2	0.00	6
	ATOM	1830	CZ	PHE	В	301	80.215	11.783	12.235	1.00 2	0.00	6
	ATOM	1831	С	PHE	В	301	80.009	5.722	9.744	1.00 2	0.00	6
35	ATOM	1832	0	PHE	В	301	79.506	4.839	10.442	1.00 2		8
	ATOM	1833	N	PRO		302	80.842	5.440	8.732	1.00 2		7
	ATOM	1834	CD	PRO		302	81.330	6.316	7.654	1.00 2		6
	ATOM	1835	CA	PRO		302	81.191	4.044	8.466	1.00 2		6
	ATOM	1836	CB	PRO		302	81.838	4.105	7.084	1.00 2		6
40	ATOM	1837	CG	PRO		302	82.425	5.479	7.046	1.00 2		6
40									9.569			
	ATOM	1838	С	PRO		302	82.168	3.629		1.00 2		6
	MOTA	1839	0	PRO		302	82.887	4.469	10.111	1.00 2		8
	MOTA	1840	N	ALA		303	82.185	2.345	9.908	1.00 2		7
	MOTA	1841	CA	ALA		303	83.052	1.836	10.968	1.00 2		6
45	MOTA	1842	CB	ALA		303	82.993	0.310	10.987	1.00 2		6
	MOTA	1843	C	ALA		303	84.513	2.294	10.939	1.00 2		6
	MOTA	1844	0	ALA	В	303	85.078	2.637	11.979	1.00 2	0.00	8
	MOTA	1845	N	ALA	В	304	85.121	2.306	9.756	1.00 2	0.00	7
	MOTA	1846	CA	ALA	В	304	86.527	2.684	9.605	1.00 2	0.00	6
50	MOTA	1847	CB	ALA	В	304	86.971	2.423	8.165	1.00 2	0.00	6
	ATOM	1848	С	ALA	В	304	86.894	4.119	10.001	1.00 2	0.00	6
	ATOM	1849	ō	ALA		304	87.983	4.367	10.520	1.00 2		8
	ATOM	1850	N	PHE		305	85.985	5.053	9.742	1.00 2		7
	ATOM	1851	CA	PHE		305	86.183	6.473	10.034	1.00 2		6
55	ATOM	1852	CB	PHE		305	84.822	7.115	10.312	1.00 2		6
55	ATOM	1853	CG	PHE		305	84.705	8.522	9.815	1.00 2		6
	ATOM	1853		PHE		305		9.572	10.502	1.00 2		
							85.303					6
	MOTA	1855		PHE		305	84.003	8.800	8.646	1.00 2		6
	ATOM	1856	CE1	PHE	В	305	85.202	10.881	10.033	1.00 2	U.00	6

	MOTA	1857	CE2	PHE	В	305	83.896	10.106	8.167	1.00 20.	0.0	6
	ATOM	1858	CZ	PHE		305	84.496	11.147	8.862	1.00 20.		6
	ATOM	1859	C	PHE		305	87.153	6.789	11.182	1.00 20.		6
	ATOM	1860	ō	PHE		305	86.964	6.342	12.312	1.00 20.		8
5	ATOM	1861	N	PHE		306	88.190	7.565	10.883	1.00 20.		7
,	MOTA	1862	CA	PHE		306	89.176	7.945	11.894	1.00 20.		6
	ATOM	1863	CB	PHE		306	90.179	8.936	11.295	1.00 20.		6
	ATOM	1864	CG	PHE		306	90.695	8.531	9.940	1.00 20.		6
	ATOM	1865		PHE		306	91.292	7.284	9.747	1.00 20.		6
10												
10	ATOM	1866	CD2			306	90.588	9.395	8.853	1.00 20.		6
	MOTA	1867	CE1			306	91.774	6.906	8.490	1.00 20.		6
	MOTA	1868		PHE		306	91.067	9.027	7.590	1.00 20.		6
	MOTA	1869	CZ	PHE		306	91.662	7.780	7.408	1.00 20.		6
	ATOM	1870	С	PHE		306	88.445	8.575	13.086	1.00 20.		6
15	MOTA	1871	0	PHE		306	87.731	9.566	12.936	1.00 20.		8
	ATOM	1872	N	PRO	В	307	88.614	7.995	14.288	1.00 20.	00	7
	MOTA	1873	CD	PRO	В	307	89.482	6.834	14.555	1.00 20.	00	6
	ATOM	1874	CA	PRO	В	307	87.983	8.459	15.530	1.00 20.	0.0	6
	ATOM	1875	CB	PRO	В	307	88.748	7.691	16.606	1.00 20.	0.0	6
20	ATOM	1876	CG	PRO	В	307	89.018	6.388	15.928	1.00 20.	0.0	6
	ATOM	1877	C	PRO	В	307	87.986	9.965	15.784	1.00 20.	0.0	6
	MOTA	1878	0	PRO	В	307	86.936	10.565	16.025	1.00 20.	00	8
	ATOM	1879	N	LYS		308	89.162	10.575	15.745	1.00 20.		7
	ATOM	1880	CA	LYS		308	89.260	12.004	15.992	1.00 20.		6
25	ATOM	1881	CB	LYS		308	90.728	12.405	16.149	1.00 20.		6
	ATOM	1882	CG	LYS		308	91.338	11.805	17.410	1.00 20.		6
	ATOM	1883	CD	LYS		308	92.806	12.140	17.591	1.00 20.		6
	ATOM	1884	CE	LYS		308	93.339	11.457	18.847	1.00 20.		6
	ATOM	1885	NZ	LYS		308	94.816	11.573	18.985	1.00 20.		7
30	ATOM	1886	C	LYS		308	88.572	12.808	14.894	1.00 20.		6
30	ATOM	1886		LYS		308	87.985	13.855	15.167	1.00 20.		8
			0									
	ATOM	1888	N	ALA		309	88.629	12.318	13.659	1.00 20.		7
	MOTA	1889	CA	ALA		309	87.967	13.011	12.557	1.00 20.		6
	MOTA	1890	CB	ALA		309	88.328	12.369	11.231	1.00 20.		6
35	MOTA	1891	C	ALA		309	86.460	12.936	12.787	1.00 20.		6
	MOTA	1892	0	ALA		309	85.735	13.903	12.552	1.00 20.		8
	ATOM	1893	N	ARG		310	85.986	11.780	13.246	1.00 20.		7
	MOTA	1894	CA	ARG		310	84.561	11.619	13.513	1.00 20.		6
	MOTA	1895	CB	ARG		310	84.246	10.194	13.979	1.00 20.		6
40	MOTA	1896	CG	ARG	В	310	82.844	10.069	14.561	1.00 20.	00	6
	MOTA	1897	CD	ARG	В	310	82.408	8.632	14.789	1.00 20.	00	6
	MOTA	1898	NE	ARG	В	310	81.060	8.593	15.355	1.00 20.	00	7
	ATOM	1899	CZ	ARG	В	310	80.259	7.532	15.328	1.00 20.	00	6
	ATOM	1900	NH1	ARG	В	310	80.665	6.401	14.759	1.00 20.	00	7
45	ATOM	1901	NH2	ARG	В	310	79.048	7.601	15.867	1.00 20.	00	7
	MOTA	1902	C	ARG	В	310	84.110	12.613	14.583	1.00 20.	0.0	6
	ATOM	1903	0	ARG	В	310	83.080	13.274	14.436	1.00 20.	0.0	8
	ATOM	1904	N	ASP		311	84.876	12.707	15.666	1.00 20.		7
	ATOM	1905	CA	ASP		311	84.535	13.629	16.740	1.00 20.		6
50	ATOM	1906	CB	ASP		311	85.574	13.555	17.864	1.00 20.		6
50	ATOM	1907	CG	ASP		311	85.260	14.505	19.006	1.00 20.		6
	ATOM	1908		ASP		311	85.782	15.636	19.010	1.00 20.		8
	MOTA	1909		ASP		311	84.480	14.124	19.901	1.00 20.		8
	ATOM	1910	C	ASP		311	84.445	15.054	16.198	1.00 20.		6
55	ATOM	1910	0	ASP		311	83.539	15.800	16.198	1.00 20.		8
23												
	MOTA	1912	N	LEU		312	85.371	15.423	15.313	1.00 20.		7
	MOTA	1913	CA	LEU		312	85.362	16.769	14.736	1.00 20.		6
	MOTA	1914	CB	LEU		312	86.604	16.999	13.869	1.00 20.		6
	MOTA	1915	CG	LEU	В	312	86.662	18.329	13.099	1.00 20.	υ0	6

	MOTA	1916	CD1	LEU	В	312	86.424	19.510	14.037	1.00	20.00	6
	MOTA	1917	CD2	LEU	В	312	88.018	18.450	12.414	1.00	20.00	6
	MOTA	1918	C	LEU	В	312	84.112	17.008	13.899	1.00	20.00	6
	ATOM	1919	0	LEU	В	312	83.456	18.039	14.035	1.00	20.00	8
5	ATOM	1920	N	VAL	В	313	83.786	16.051	13.033	1.00	20.00	7
	MOTA	1921	CA	VAL		313	82.611	16.171	12.183		20.00	6
	ATOM	1922	CB	VAL		313	82.464	14.942	11.255		20.00	6
	ATOM	1923		VAL		313	81.121	14.973	10.551		20.00	6
	ATOM	1924	CG2			313	83.595	14.935	10.228		20.00	6
10	ATOM	1925	C	VAL		313	81.354	16.315	13.036		20.00	6
	ATOM	1926	ō	VAL		313	80.467	17.111	12.716		20.00	8
	ATOM	1927	N	GLU		314	81.282	15.559	14.129		20.00	7
	ATOM	1928	CA	GLU		314	80.122	15.634	15.010		20.00	6
	ATOM	1929	CB	GLU		314	80.191	14.545	16.084		20.00	6
15	ATOM	1930	CG	GLU		314	80.160	13.131	15.521		20.00	6
13	ATOM	1931	CD	GLU		314	80.222	12.073	16.603		20.00	6
												8
	ATOM	1932		GLU		314	81.033	12.227	17.542		20.00	
	ATOM	1933		GLU		314	79.469	11.081	16.512		20.00	8
20	ATOM	1934 1935	C	GLU		314 314	80.035	17.005	15.664		20.00	6
20	ATOM			GLU			78.960	17.443	16.059		20.00	8
	ATOM	1936	N	LYS		315	81.165	17.690	15.776		20.00	7
	MOTA	1937	CA	LYS		315	81.154	19.010	16.383		20.00	6
	MOTA	1938	CB	LYS		315	82.448	19.240	17.168		20.00	6
	MOTA	1939	CG	LYS		315	82.460	18.478	18.493		20.00	6
25	MOTA	1940	CD	LYS		315	83.803	18.529	19.198		20.00	6
	MOTA	1941	CE	LYS		315	83.749	17.825	20.552		20.00	6
	MOTA	1942	NZ	LYS		315	82.829	18.505	21.506		20.00	7
	MOTA	1943	С	LYS		315	80.934	20.104	15.343		20.00	6
	MOTA	1944	0	LYS		315	80.855	21.282	15.686		20.00	8
30	MOTA	1945	N	LEU		316	80.819	19.706	14.075		20.00	7
	MOTA	1946	CA	LEU		316	80.577	20.649	12.979		20.00	6
	MOTA	1947	CB	LEU	В	316	81.608	20.450	11.863	1.00	20.00	6
	MOTA	1948	CG	LEU	В	316	83.044	20.833	12.240	1.00	20.00	6
	MOTA	1949	CD1	LEU	В	316	84.011	20.365	11.156	1.00	20.00	6
35	MOTA	1950	CD2	LEU	В	316	83.124	22.351	12.434	1.00	20.00	6
	MOTA	1951	C	LEU	В	316	79.164	20.469	12.415	1.00	20.00	6
	MOTA	1952	0	LEU	В	316	78.464	21.448	12.148	1.00	20.00	8
	MOTA	1953	N	LEU	В	317	78.746	19.220	12.230	1.00	20.00	7
	ATOM	1954	CA	LEU	В	317	77.403	18.962	11.721	1.00	20.00	6
40	MOTA	1955	CB	LEU	В	317	77.343	17.605	11.012	1.00	20.00	6
	MOTA	1956	CG	LEU	В	317	78.335	17.445	9.852	1.00	20.00	6
	MOTA	1957	CD1	LEU	В	317	78.091	16.111	9.143	1.00	20.00	6
	ATOM	1958	CD2	LEU	В	317	78.182	18.603	8.866	1.00	20.00	6
	ATOM	1959	С	LEU	В	317	76.435	19.000	12.899	1.00	20.00	6
45	ATOM	1960	0	LEU	В	317	75.979	17.966	13.398	1.00	20.00	8
	MOTA	1961	N	VAL	В	318	76.156	20.215	13.354	1.00	20.00	7
	ATOM	1962	CA	VAL	В	318	75.251	20.451	14.467	1.00	20.00	6
	ATOM	1963	CB	VAL	В	318	75.981	21.164	15.625	1.00	20.00	6
	ATOM	1964		VAL		318	75.007	21.461	16.759		20.00	6
50	ATOM	1965	CG2			318	77.136	20.300	16.115		20.00	6
	MOTA	1966	С	VAL		318	74.140	21.344	13.936		20.00	6
	ATOM	1967	o	VAL		318	74.410	22.386	13.333		20.00	8
	ATOM	1968	N	LEU		319	72.892	20.941	14.153		20.00	7
	ATOM	1969	CA	LEU		319	71.758	21.717	13.663		20.00	6
55	ATOM	1970	CB	LEU		319	70.444	21.056	14.093		20.00	6
	ATOM	1971	CG	LEU		319	70.211	19.647	13.533		20.00	6
	ATOM	1972		LEU		319	68.883	19.098	14.060		20.00	6
	ATOM	1973		LEU		319	70.211	19.688	12.000		20.00	6
	ATOM	1974	CDZ	LEU		319	71.794	23.173	14.119	1.00		6
	111 011	1214	_	200	ъ	- L -	11.134		-4.113	4.00		0

	MOTA	1975	0	LEU			71.591	24.082	13.317		20.00	8
	ATOM	1976	N	ASP	В	320	72.052	23.394	15.405		20.00	7
	MOTA	1977	CA	ASP	В	320	72.119	24.745	15.958	1.00	20.00	6
	MOTA	1978	CB	ASP	В	320	72.091	24.687	17.490	1.00	20.00	6
5	ATOM	1979	CG	ASP	В	320	72.058	26.061	18.129	1.00	20.00	6
	MOTA	1980	OD1	ASP	В	320	72.506	27.036	17.492	1.00	20.00	8
	ATOM	1981	OD2	ASP	В	320	71.595	26.166	19.284	1.00	20.00	8
	ATOM	1982	C	ASP	В	320	73.415	25.419	15.492	1.00	20.00	6
	ATOM	1983	0	ASP			74.496	25.089	15.965		20.00	8
10	ATOM	1984	N	ALA			73.294	26.372	14.576		20.00	7
	ATOM	1985	CA	ALA			74.450	27.078	14.028		20.00	6
	ATOM	1986	CB	ALA			73.982	28.109	13.006		20.00	6
	ATOM	1987	C	ALA			75.359	27.747	15.065		20.00	6
	ATOM	1988	ō	ALA			76.535	27.992	14.790		20.00	8
15	ATOM	1989	N	THR		322	74.829	28.035	16.252		20.00	7
	ATOM	1990	CA	THR		322	75.631	28.681	17.292		20.00	6
	ATOM	1991	CB	THR			74.755	29.491	18.271		20.00	6
	ATOM	1992		THR			73.879	28.605	18.973		20.00	8
	ATOM	1993	CG2				73.928	30.527	17.519		20.00	6
20	ATOM	1994	C	THR		322	76.437	27.684	18.108		20.00	6
20	ATOM	1995	Ö	THR		322	77.166	28.071	19.019		20.00	8
	ATOM	1996	N	LYS	В		76.312	26.401	17.786		20.00	7
	ATOM	1997	CA	LYS		323	77.048	25.378	18.517		20.00	6
	ATOM	1998	CB	LYS	В	323	76.080	24.378	19.155	1.00		6
25	ATOM	1999	CG	LYS	В	323	75.180	24.992	20.209	1.00		6
20	ATOM	2000	CD	LYS			74.356	23.931	20.924	1.00		6
	ATOM	2001	CE	LYS		323	73.406	24.574	21.927		20.00	6
	ATOM	2002	NZ	LYS		323	74.144	25.514	22.818	1.00		7
	ATOM	2003	C	LYS		323	78.066	24.631	17.664		20.00	6
30	ATOM	2004	ŏ	LYS		323	78.520	23.557	18.040		20.00	8
50	ATOM	2005	N	ARG		324	78.427	25.195	16.517		20.00	7
	ATOM	2006	CA	ARG		324	79.408	24.545	15.656	1.00		6
	ATOM	2007	CB	ARG		324	79.108	24.834	14.186		20.00	6
	ATOM	2008	CG	ARG			77.824	24.177	13.728		20.00	6
35	ATOM	2009	CD	ARG		324	77.468	24.505	12.297		20.00	6
	ATOM	2010	NE	ARG			76.060	24.202	12.069		20.00	7
	ATOM	2011	CZ	ARG			75.277	24.873	11.233		20.00	6
	ATOM	2012		ARG			75.764	25.888	10.523		20.00	7
	ATOM	2013		ARG		324	73.992	24.551	11.140		20.00	7
40	ATOM	2014	C	ARG			80.811	25.011	16.008		20.00	6
	ATOM	2015	ō	ARG			81.070	26.212	16.131		20.00	8
	ATOM	2016	N	LEU			81.711	24.049	16.180		20.00	7
	ATOM	2017	CA	LEU			83.090	24.350	16.520		20.00	6
	ATOM	2018	CB	LEU			83.913	23.061	16.550		20.00	6
45	ATOM	2019	CG	LEU			85.274	23.123	17.241		20.00	6
	ATOM	2020		LEU			85.093	23.591	18.682		20.00	6
	ATOM	2021		LEU			85.922	21.741	17,209		20.00	6
	ATOM	2022	C	LEU			83.656	25.310	15.481		20.00	6
	ATOM	2023	0	LEU			83.649	25.015	14.282		20.00	8
50	ATOM	2024	N	GLY		326	84.139	26.461	15.946		20.00	7
	MOTA	2025	CA	GLY	В	326	84.697	27.449	15.040	1.00	20.00	6
	MOTA	2026	C	GLY	В	326	83.857	28.711	14.932	1.00	20.00	6
	ATOM	2027	ō	GLY			84.369	29.757	14.529	1.00		8
	ATOM	2028	N	CYS		327	82.575	28.632	15.286		20.00	7
55	ATOM	2029	CA	CYS		327	81.714	29.806	15.200		20.00	6
	MOTA	2030	CB	CYS	В	327	80.233	29.404	15.183	1.00	20.00	6
	MOTA	2031	SG	CYS	В	327	79.534	28.915	16.774	1.00		16
	MOTA	2032	C	CYS	В	327	81.976	30.772	16.353	1.00	20.00	6
	MOTA	2033	0	CYS	В	327	82.565	30.410	17.371	1.00	20.00	8

	MOTA	2034	N	GLU			81.523	32.005	16.178		20.00	7
	MOTA	2035	CA	GLU		328	81.714	33.052	17.167		20.00	6
	MOTA	2036	CB	GLU		328	81.087	34.348	16.632		20.00	6
	MOTA	2037	CG	GLU	В	328	81.734	34.772	15.300	1.00	20.00	6
5	ATOM	2038	CD	GLU	В	328	80.962	35.842	14.539	1.00	20.00	6
	MOTA	2039	OE1	GLU	В	328	79.738	35.676	14.343	1.00	20.00	8
	ATOM	2040	OE2	GLU	В	328	81.588	36.840	14.116	1.00	20.00	8
	ATOM	2041	С	GLU	В	328	81.187	32.701	18.560	1.00	20.00	6
	ATOM	2042	o	GLU	В	328	81.850	32.983	19.562		20.00	8
10	ATOM	2043	N	GLU		329	80.016	32.073	18.631		20.00	7
	ATOM	2044	CA	GLU		329	79.449	31.714	19.926		20.00	6
	ATOM	2045	CB	GLU		329	77.991	31.263	19.782		20.00	6
	ATOM	2046	CG	GLU		329	77.028	32.355	19.315		20.00	6
	ATOM	2047	CD	GLU		329	77.055	32.575	17.813		20.00	6
15	ATOM	2048		GLU		329	77.859	31.910	17.120	1.00		8
	ATOM	2049		GLU		329	76.267	33.413	17.323		20.00	8
	ATOM	2050	C	GLU		329	80.264	30.616	20.605		20.00	6
	ATOM	2051	ō	GLU		329	80.182	30.436	21.819		20.00	8
	ATOM	2051	N	MET		330	81.040	29.878	19.816		20.00	7
20		2052	CA	MET		330	81.880	28.813	20.354		20.00	
20	ATOM	2053	CB	MET			81.872	27.600	19.419		20.00	6
	ATOM					330						
	ATOM	2055	CG	MET			80.552	26.822	19.436		20.00	6
	MOTA	2056	SD	MET		330	80.117	26.254	21.104		20.00	
2.5	ATOM	2057	CE			330	81.265	24.895	21.311		20.00	6
25	ATOM	2058	С	MET			83.302	29.330	20.547		20.00	6
	ATOM	2059	0	MET		330	84.236	28.564	20.754		20.00	8
	MOTA	2060	N	GLU		331	83.443	30.647	20.471		20.00	7
	MOTA	2061	CA	GLU		331	84.716	31.338	20.656		20.00	6
	MOTA	2062	CB	GLU		331	85.357	30.921	21.987		20.00	6
30	MOTA	2063	CG	GLU		331	84.371	30.886	23.163		20.00	6
	MOTA	2064	CD	GLU		331	83.478	32.127	23.270		20.00	6
	ATOM	2065		GLU		331	82.483	32.064	24.021	1.00	20.00	8
	ATOM	2066		GLU		331	83.759	33.159	22.625		20.00	8
	ATOM	2067	С	GLU	В	331	85.742	31.247	19.523	1.00	20.00	6
35	ATOM	2068	0	GLU	В	331	86.952	31.264	19.761	1.00	20.00	8
	ATOM	2069	N	GLY	В	332	85.257	31.137	18.292	1.00	20.00	7
	MOTA	2070	CA	GLY	В	332	86.145	31.159	17.140	1.00	20.00	6
	MOTA	2071	C	GLY	В	332	87.036	30.014	16.721	1.00	20.00	6
	MOTA	2072	0	GLY	В	332	86.881	28.863	17.142	1.00	20.00	8
40	MOTA	2073	N	TYR	В	333	88.002	30.366	15.875	1.00	20.00	7
	MOTA	2074	CA	TYR	В	333	88.939	29.413	15.307	1.00	20.00	6
	ATOM	2075	CB	TYR	В	333	89.625	30.053	14.093	1.00	20.00	6
	ATOM	2076	CG	TYR	В	333	88.724	30.031	12.877	1.00	20.00	6
	ATOM	2077	CD1	TYR	В	333	88.774	28.966	11.974	1.00	20.00	6
45	ATOM	2078	CE1	TYR	В	333	87.872	28.869	10.919	1.00	20.00	6
	ATOM	2079	CD2	TYR	В	333	87.747	31.011	12.686	1.00	20.00	6
	ATOM	2080	CE2	TYR	В	333	86.831	30.923	11.624	1.00	20.00	6
	ATOM	2081	CZ	TYR	В	333	86.903	29.845	10.751	1.00	20.00	6
	ATOM	2082	OH	TYR	В	333	86.001	29.719	9.724	1.00	20.00	8
50	ATOM	2083	С	TYR		333	89.958	28.800	16.252		20.00	6
	ATOM	2084	0	TYR		333	90.473	27.721	15.971		20.00	8
	ATOM	2085	N	GLY		334	90.242	29.469	17.369	1.00		7
	ATOM	2086	CA	GLY		334	91,193	28.921	18.327		20.00	6
	ATOM	2087	C	GLY		334	90.803	27.504	18.741	1.00		6
55	ATOM	2088	ō	GLY		334	91.577	26.564	18.558	1.00	20.00	8
	ATOM	2089	N	PRO		335	89.603	27.320	19.309	1.00		7
	ATOM	2090	CD	PRO		335	88.703	28.372	19.814	1.00		6
	ATOM	2091	CA	PRO		335	89.145	25.991	19.731		20.00	6
	ATOM	2091	CB	PRO		335	87.759	26.275	20.303		20.00	6
	ALCH	2002	CD	2100	ъ		01.133			1.00		0

	ATOM	2093	CG	PRO	В	335	87.925	27.644	20.883	1.00 20.00	6
	ATOM	2094	C	PRO	В	335	89.104	24.986	18.573	1.00 20.00	6
	ATOM	2095	0	PRO		335	89.406	23.808	18.756	1.00 20.00	
	ATOM	2096	N	LEU		336	88.727	25.450	17.382	1.00 20.00	
5	ATOM	2097	CA	LEU		336	88.666	24.567	16.219	1.00 20.00	
-	ATOM	2098	CB	LEU		336	88.031	25.292	15.023	1.00 20.00	
	ATOM	2099	CG	LEU		336	88.051	24.581	13.663	1.00 20.00	
	ATOM	2100		LEU		336	87.486	23.177	13.787	1.00 20.00	
	ATOM	2101	CD2	LEU			87.239	25.399	12.653	1.00 20.00	
10	ATOM	2101	CDZ	LEU		336	90.060	24.068	15.839	1.00 20.00	
10											
	ATOM	2103	0	LEU		336	90.274	22.870	15.665	1.00 20.00	
	ATOM	2104	N	LYS		337	91.011	24.986	15.717	1.00 20.00	
	MOTA	2105	CA	LYS	В	337	92.370	24.597	15.360	1.00 20.00	
	ATOM	2106	CB	LYS		337	93.198	25.848	15.046	1.00 20.00	
15	MOTA	2107	CG	LYS	В	337	92.678	26.560	13.801	1.00 20.00	
	ATOM	2108	CD	LYS		337	93.111	28.014	13.717	1.00 20.00	
	MOTA	2109	CE	LYS		337	94.561	28.167	13.314	1.00 20.00	
	MOTA	2110	NZ	LYS		337	94.882	29.611	13.122	1.00 20.00	
	MOTA	2111	С	LYS		337	93.020	23.764	16.467	1.00 20.00	
20	MOTA	2112	0	LYS		337	93.965	23.015	16.215	1.00 20.00	
	ATOM	2113	N	ALA	В	338	92.495	23.866	17.684	1.00 20.00	7
	MOTA	2114	CA	ALA	В	338	93.056	23.105	18.799	1.00 20.00	6
	ATOM	2115	CB	ALA	В	338	92.873	23.877	20.105	1.00 20.00	6
	ATOM	2116	С	ALA	В	338	92.441	21.718	18.929	1.00 20.00	6
25	ATOM	2117	0	ALA	В	338	92.805	20.955	19.820	1.00 20.00	- 8
	ATOM	2118	N	HIS	В	339	91.513	21.375	18.043	1.00 20.00	7
	ATOM	2119	CA	HIS	В	339	90.886	20.061	18.129	1.00 20.00	6
	ATOM	2120	CB	HIS	В	339	89.786	19.919	17.074	1.00 20.00	6
	ATOM	2121	CG	HIS	В	339	88.999	18.654	17.199	1.00 20.00	6
30	ATOM	2122	CD2	HIS	В	339	87.797	18.406	17.774	1.00 20.00	6
	ATOM	2123		HIS		339	89.462	17.440	16.737	1.00 20.00	
	ATOM	2124		HIS		339	88.578	16.498	17.021	1.00 20.00	
	ATOM	2125		HIS		339	87.559	17.057	17.650	1.00 20.00	
	ATOM	2126	C	HIS		339	91.928	18.952	17.970	1.00 20.00	
35	ATOM	2127	ō	HIS		339	92.863	19.077	17.186	1.00 20.00	
-	ATOM	2128	N	PRO		340	91.780	17.854	18.731	1.00 20.00	
	ATOM	2129	CD	PRO		340	90.747	17.655	19.765	1.00 20.00	
	ATOM	2130	CA	PRO		340	92.700	16.711	18.694	1.00 20.00	
	ATOM	2131	CB	PRO		340	91.966	15.665	19.521	1.00 20.00	
40	ATOM	2132	CG	PRO		340	91.310	16.505	20.579	1.00 20.00	
40	ATOM	2133	C	PRO		340	93.072	16.198	17.301	1.00 20.00	
	ATOM	2134	Ö	PRO		340	94.193	15.748	17.080	1.00 20.00	
	ATOM	2135	N		В	341	92.139	16.270	16.362	1.00 20.00	
	ATOM	2136	CA	PHE		341	92.407	15.797	15.011	1.00 20.00	
45		2137	CB		В	341				1.00 20.00	
43	ATOM		CG	PHE			91.152	15.943	14.142		
	ATOM	2138				341	91.317	15.424	12.738	1.00 20.00	
	ATOM	2139				341	91.596	14.080	12.507	1.00 20.00	
	ATOM	2140		PHE		341	91.182	16.277	11.647	1.00 20.00	
50	ATOM	2141		PHE		341	91.738	13.592	11.207	1.00 20.00	
30	ATOM	2142		PHE			91.320	15.803	10.345	1.00 20.00	
	MOTA	2143	CZ			341	91.599	14.457	10.123	1.00 20.00	
	ATOM	2144	C			341	93.571	16.550	14.362	1.00 20.00	
	MOTA	2145	0	PHE		341	94.268	16.002	13.514	1.00 20.00	
	MOTA	2146	N	PHE		342	93.777	17.800	14.765	1.00 20.00	
55	MOTA	2147	CA		В	342	94.842	18.630	14.202	1.00 20.00	
	MOTA	2148	CB	PHE		342	94.336	20.058	13.975	1.00 20.00	
	MOTA	2149	CG	PHE	В	342	93.124	20.152	13.096	1.00 20.00	
	MOTA	2150		PHE		342	93.166	19.729	11.777	1.00 20.00	
	MOTA	2151	CD2	PHE	В	342	91.954	20.734	13.575	1.00 20.00	6

	ATOM	2152	CE1	PHE	В	342	92.058	19.888	10.936	1.00 20.0	0 6
	ATOM	2153	CE2	PHE	В	342	90.843	20.898	12.742	1.00 20.0	0 6
	ATOM	2154	CZ			342	90.898	20.475	11.423	1.00 20.0	
	ATOM	2155	c	PHE		342	96.077	18.718	15.101	1.00 20.0	
5	ATOM	2156	ō			342	96.932	19.584	14.902	1.00 20.0	
-	ATOM	2157	N	GLU			96.173	17.829	16.083	1.00 20.0	
	ATOM	2158	CA	GLU		343	97.293	17.857	17.022	1.00 20.0	
	ATOM	2159	CB	GLU		343	97.330	16.564	17.841	1.00 20.0	
		2160	CG	GLU		343	98.475	16.525	18.839	1.00 20.0	
10	ATOM										
10	MOTA	2161	CD	GLU		343	98.372	15.365	19.813	1.00 20.0	
	ATOM	2162	OE1	GLU		343	98.290	14.201	19.359	1.00 20.0	
	MOTA	2163	OE2	GLU		343	98.379	15.622	21.036	1.00 20.0	
	MOTA	2164	С	GLU		343	98.683	18.113	16.430	1.00 20.0	
	MOTA	2165	0	GLU		343	99.419	18.969	16.925	1.00 20.0	
15	MOTA	2166	N	SER		344	99.047	17.382	15.383	1.00 20.0	
	ATOM	2167	CA	SER		344	100.370	17.549	14.781	1.00 20.0	0 6
	MOTA	2168	CB	SER	В	344	100.848	16.219	14.192	1.00 20.0	0 6
	ATOM	2169	OG	SER	В	344	100.072	15.856	13.065	1.00 20.0	0 8
	ATOM	2170	C	SER	В	344	100.467	18.629	13.702	1.00 20.0	0 6
20	ATOM	2171	0	SER	В	344	101.485	18.732	13.025	1.00 20.0	0 8
	ATOM	2172	N	VAL	В	345	99.423	19.435	13.544	1.00 20.0	0 7
	ATOM	2173	CA	VAL	В	345	99.430	20.486	12.527	1.00 20.0	0 6
	ATOM	2174	CB		В	345	97.985	20.843	12.075	1.00 20.0	
	ATOM	2175		VAL		345	98.015	22.042	11.120	1.00 20.0	
25	ATOM	2176		VAL		345	97.335	19.646	11.400	1.00 20.0	
	ATOM	2177	c	VAL		345	100.096	21.785	12.980	1.00 20.0	
	ATOM	2178	ō	VAL		345	99.844	22.275	14.085	1.00 20.0	
	ATOM	2179	N	THR		346	100.951	22.335	12.122	1.00 20.0	
	ATOM	2180	CA	THR		346	101.602	23.610	12.397	1.00 20.0	
30	ATOM	2181	CB	THR		346	103.096	23.593	11.982	1.00 20.0	
30	ATOM	2182		THR		346	103.096	22.688	12.831	1.00 20.0	
								24.983			
	ATOM	2183	CG2	THR		346	103.707		12.115	1.00 20.0	
	ATOM	2184	С	THR			100.810	24.573	11.510	1.00 20.0	
	ATOM	2185	0	THR		346	100.950	24.565	10.285	1.00 20.0	
35	ATOM	2186	N	TRP		347	99.966	25.385	12.138	1.00 20.0	
	ATOM	2187	CA	TRP		347	99.089	26.306	11.425	1.00 20.0	
	MOTA	2188	CB	TRP		347	97.941	26.727	12.344	1.00 20.0	
	MOTA	2189	CG	TRP		347	97.088	25.594	12.818	1.00 20.0	
	MOTA	2190		TRP		347	95.924	25.071	12.165	1.00 20.0	
40	MOTA	2191	CE2	TRP		347	95.436	24.008	12.963	1.00 20.0	
	MOTA	2192	CE3			347	95.247	25.397	10.983	1.00 20.0	
	ATOM	2193		TRP		347	97.259	24.848	13.953	1.00 20.0	
	MOTA	2194	NE1	TRP	В	347	96.269	23.893	14.048	1.00 20.0	0 7
	ATOM	2195	CZ2	TRP	В	347	94.300	23.270	12.616	1.00 20.0	0 6
45	ATOM	2196	CZ3	TRP	В	347	94.113	24.661	10.636	1.00 20.0	0 6
	MOTA	2197	CH2	TRP	В	347	93.654	23.610	11.452	1.00 20.0	0 6
	ATOM	2198	C	TRP	В	347	99.679	27.563	10.800	1.00 20.0	0 6
	ATOM	2199	0	TRP	В	347	99.101	28.114	9.867	1.00 20.0	0 8
	MOTA	2200	N	ALA		348	100.820	28.016	11.308	1.00 20.0	
50	ATOM	2201	CA	ALA		348	101.439	29.247	10.822	1.00 20.0	
	MOTA	2202	СВ	ALA		348	102.582	29.656	11.761	1.00 20.0	
	ATOM	2203	C	ALA		348	101.933	29.277	9.381	1.00 20.0	
	ATOM	2204	ŏ	ALA		348	101.874	30.323	8.738	1.00 20.0	
	ATOM	2205	N	ASN		349	102.411	28.152	8.860	1.00 20.0	
55	ATOM	2206	CA	ASN		349	102.940	28.153	7.500	1.00 20.0	
55	ATOM	2206	CB	ASN		349	104.466	28.205	7.569	1.00 20.0	
	ATOM	2207	CG	ASN	В	349	105.058	26.929	8.138	1.00 20.0	
	ATOM	2200		ASN		349	104.445	26.282	8.984	1.00 20.0	
		2210		ASN		349				1.00 20.0	
	ATOM	2210	ND2	ASN	25	349	106.251	26.563	7.678	1.00 ∠0.0	10 /

	ATOM	2211	C	ASN	В	349	102.522	26.966	6.634	1.00	20.00	6
	MOTA	2212	0	ASN	В	349	103.353	26.371	5.944	1.00	20.00	8
	MOTA	2213	N	LEU	В	350	101.242	26.628	6.643	1.00	20.00	7
	ATOM	2214	CA	LEU	В	350	100.776	25.500	5.846		20.00	6
5	ATOM	2215	CB	LEU			99.257	25.355	5.973		20.00	6
	ATOM	2216	CG	LEU			98.734	24.848	7.316		20.00	6
	ATOM	2217		LEU		350	97.244	25.127	7.418		20.00	6
	MOTA	2218		LEU		350	99.030	23.357	7.444		20.00	6
	MOTA	2219	С	LEU			101.147	25.574	4.365		20.00	6
10	MOTA	2220	0	LEU		350	101.557	24.575	3.775		20.00	8
	MOTA	2221	N	HIS		351	101.006	26.744	3.752		20.00	7
	ATOM	2222	CA	HIS		351	101.305	26.829	2.329		20.00	6
	MOTA	2223	CB	HIS	В	351	100.651	28.087	1.721	1.00	20.00	6
	ATOM	2224	CG	HIS	В	351	101.553	29.274	1.618	1.00	20.00	6
15	MOTA	2225	CD2	HIS	В	351	102.001	30.143	2.556	1.00	20.00	6
	ATOM	2226	ND1	HIS	В	351	102.072	29.706	0.416	1.00	20.00	7
	MOTA	2227	CE1	HIS	В	351	102.798	30.792	0.618	1.00	20.00	6
	ATOM	2228		HIS		351	102.772	31.079	1.907		20.00	7
	ATOM	2229	С	HIS		351	102.797	26.731	1.999		20.00	6
20	ATOM	2230	ō	HIS		351	103.176	26.669	0.832		20.00	8
	ATOM	2231	N	GLN		352	103.634	26.685	3.033		20.00	7
	ATOM	2232	CA	GLN		352	105.081	26.554	2.851		20.00	6
	ATOM	2233	CB	GLN		352	105.841	27.458	3.819		20.00	6
		2233	CG	GLN			106.395	28.705	3.166		20.00	6
25	ATOM	2234	CD	GLN		352	105.930	29.966	3.854		20.00	6
23	ATOM											
	MOTA	2236		GLN		352	106.134	30.139	5.053		20.00	8
	MOTA	2237		GLN		352	105.299	30.854	3.096		20.00	7
	MOTA	2238	С	GLN			105.478	25.099	3.088		20.00	6
	MOTA	2239	0	GLN		352	106.632	24.715	2.895		20.00	8
30	MOTA	2240	N	GLN		353	104.514	24.295	3.522		20.00	7
	ATOM	2241	CA	GLN	В	353	104.761	22.888	3.777	1.00	20.00	6
	MOTA	2242	CB	GLN	В	353	103.849	22.395	4.900	1.00	20.00	6
	ATOM	2243	CG	GLN	В	353	104.122	23.050	6.240	1.00	20.00	6
	ATOM	2244	CD	GLN	В	353	103.075	22.711	7.281	1.00	20.00	6
35	ATOM	2245	OE1	GLN	В	353	102.627	21.571	7.377	1.00	20.00	8
	ATOM	2246	NE2	GLN	В	353	102.690	23.700	8.076		20.00	7
	ATOM	2247	С	GLN	В	353	104.507	22.079	2.510	1.00	20.00	6
	ATOM	2248	0	GLN		353	103.732	22.490	1.641		20.00	8
	ATOM	2249	N	THR		354	105.172	20.937	2.401		20.00	7
40	ATOM	2250	CA	THR		354	104.998	20.071	1.244		20.00	6
	ATOM	2251	CB	THR		354	106.240	19.173	1.029		20.00	6
	ATOM	2252		THR		354	107.390	19.999	0.790		20.00	8
	ATOM	2253		THR		354	106.033	18.243	-0.166		20.00	6
45	ATOM	2254	C	THR		354	103.777	19.197	1.501		20.00	6
43	ATOM	2255	0	THR		354	103.745	18.426	2.454		20.00	8
	MOTA	2256	N	PRO		355	102.741	19.319	0.658		20.00	7
	MOTA	2257	CD	PRO		355	102.547	20.275	-0.444		20.00	6
	MOTA	2258	CA	PRO		355	101.540	18.505	0.859		20.00	6
	MOTA	2259	CB	PRO			100.616	18.967	-0.266		20.00	6
50	MOTA	2260	CG	PRO	В	355	101.039	20.387	-0.490	1.00	20.00	6
	MOTA	2261	C	PRO	В	355	101.835	17.011	0.766	1.00	20.00	6
	MOTA	2262	0	PRO	В	355	102.631	16.577	-0.065	1.00	20.00	8
	MOTA	2263	N	PRO	В	356	101.198	16.204	1.625	1.00	20.00	7
	ATOM	2264	CD	PRO		356	100.128	16.522	2.587		20.00	6
55	MOTA	2265	CA	PRO		356	101.438	14.761	1.573		20.00	6
	ATOM	2266	СВ	PRO		356	100.593	14.235	2.729		20.00	6
	ATOM	2267	CG	PRO		356	99.429	15.188	2.737		20.00	6
	ATOM	2268	C	PRO			100.960	14.244	0.222		20.00	6
	MOTA	2269	Ö	PRO			100.005	14.779	-0.346		20.00	8

	ATOM	2270	N	ALA	В	357	101.629	13.221	-0.300	1.00	20.00	7	
	ATOM	2271	CA	ALA	В	357	101.247	12.660	-1.588	1.00	20.00	6	
	MOTA	2272	CB	ALA	В	357	102.352	11.750	-2.118	1.00	20.00	6	
	ATOM	2273	C	ALA	В	357	99.948	11.883	-1.427	1.00	20.00	6	
5	ATOM	2274	0	ALA	В	357	99.808	11.074	-0.506	1.00	20.00	8	
	MOTA	2275	N	LEU	В	358	99.000	12.134	-2.323	1.00	20.00	7	
	ATOM	2276	CA	LEU	В	358	97.709	11.460	-2.278	1.00	20.00	6	
	ATOM	2277	CB	LEU	В	358	96.729	12.166	-3.217	1.00	20.00	6	
	ATOM	2278	CG	LEU	В	358	96.368	13.582	-2.766	1.00	20.00	6	
10	ATOM	2279	CD1	LEU	В	358	95.513	14.262	-3.813	1.00	20.00	6	
	MOTA	2280	CD2	LEU	В	358	95.636	13.516	-1.430	1.00	20.00	6	
	ATOM	2281	C	LEU	В	358	97.813	9.976	-2.633	1.00	20.00	6	
	ATOM	2282	0	LEU	В	358	97.918	9.614	-3.806	1.00	20.00	8	
	ATOM	2283	N	THR	В	359	97.776	9.134	-1.600	1.00	20.00	7	
15	ATOM	2284	CA	THR	В	359	97.867	7.678	-1.735	1.00	20.00	6	
	ATOM	2285	CB	THR	В	359	96.513	7.046	-2.149	1.00	20.00	6	
	ATOM	2286	OG1	THR	В	359	96.111	7.555	-3.427	1.00	20.00	8	
	ATOM	2287	CG2	THR	В	359	95.439	7.355	-1.112	1.00	20.00	6	
	ATOM	2288	С	THR	В	359	98.933	7.238	-2.736	1.00	20.00	6	
20	ATOM	2289	0	THR	В	359	99.903	7.998	-2.945	1.00	20.00	8	
	ATOM	2290	OXT	THR	В	359	98.802	6.121	-3.280	1.00	20.00	8	
	TER												
	ATOM	2291	OH2	TIP	s	1	42.566	19.118	34.302	1.00	15.09		S
	ATOM	2292	OH2	TIP	s	2	41.052	32.378	19.857	1.00	15.82		S
25	ATOM	2293	OH2	TIP	s	3	37.014	33.030	17.747	1.00	16.95		S
	ATOM	2294	OH2	TIP	s	5	45.353	24.370	18.152	1.00	16.85		S
	ATOM	2295	OH2	TIP	S	6	31.896	13.930	33.235	1.00	20.42		S
	ATOM	2296	OH2	TIP	S	7	50.351	22.781	28.249	1.00	21.14		S
	ATOM	2297	OH2	TIP	s	8	45.246	-0.589	-0.734	1.00	17.74		S
30	MOTA	2298	OH2	TIP	s	11	46.249	-0.348	-8.523	1.00	21.32		S
	MOTA	2299	OH2	TIP	s	14	45.756	11.148	29.680	1.00	21.94		S
	ATOM	2300	OH2	TIP	S	15	44.273	13.157	34.592	1.00	15.61		S
	MOTA	2301		TIP	S	17	53.598	3.722	-1.720	1.00	21.45		S
	MOTA	2302	OH2		S	18	46.049	13.087	31.565		20.35		S
35	ATOM	2303	OH2	TIP	S	19	53.422	22.401	-3.280	1.00	23.26		S
	ATOM	2304	OH2	TIP	S	20	34.587	7.922	5.383	1.00	22.58		S
	MOTA	2305	OH2	TIP	S	21	45.053	27.379	19.376		29.60		S
	MOTA	2306	OH2	TIP	S	23	28.899	36.416	28.633		31.68		S
	MOTA	2307		TIP	S	24	35.531	11.645	-8.219		23.45		S
40	ATOM	2308		TIP	S	25	47.364	28.787	19.612		23.03		S
	MOTA	2309			S	27	48.859	21.588	12.634		23.76		S
	MOTA	2310	OH2	TIP	S	29	48.805	8.920	23.626		22.23		S
	MOTA	2311		TIP	S	31	48.619	7.247	10.112		21.32		S
	MOTA	2312		TIP	S	34	44.824	28.720	15.621		25.27		S
45	MOTA	2313		TIP	S	35	26.030	12.634	13.407		21.61		S
	MOTA	2314	OH2	TIP	S	36	50.462	19.810	40.066		25.45		S
	ATOM	2315		TIP	S	37	39.631	23.510	-0.239		30.88		S
	MOTA	2316		TIP	S	40	44.734	42.655	10.346		30.84		S
	MOTA	2317		TIP	S	41	54.653	3.902	1.503		27.14		S
50	MOTA	2318	OH2	TIP	S	45	45.693	21.923	39.754		28.30		S
	MOTA	2319	OH2	TIP	S	47	47.820	16.413	7.805		25.73		S
	ATOM	2320	OH2	TIP	S	48	50.292	31.412	29.642		32.79		S
	MOTA	2321		TIP	S	49	26.056	16.646	34.827		29.80		S
	MOTA	2322	OH2		S	52	31.714	10.996	31.855		29.15		S
55	MOTA	2323	OH2		S	53	46.108	23.843	-4.299		24.21		S
	ATOM	2324	OH2	TIP	S	54	37.645	11.206	34.448		28.56		S
	ATOM	2325	OH2	TIP	S	55	26.371	28.513	12.142	1.00	32.08		S
	ATOM	2326	OH2		S	58	33.564	19.700	3.483		28.28		S
	MOTA	2327	OH2	TIP	S	64	48.295	-0.632	14.280	1.00	32.13		S

	ATOM	2328	OH2	TIP	s	65	40.064	26.036	34.324	1.00	24.17	S
	ATOM	2329	OH2	TIP	s	66	29.570	3.958	14.729	1.00	28.94	S
	ATOM	2330		TIP	S	72	60.085	11.604	6.814		38.35	S
	ATOM	2331		TIP	S	73	39.203	44.403	18.686		26.61	s
5	ATOM	2332		TIP	s	76	47.312	12.366	27.366		28.51	S
-	MOTA	2333		TIP	s	80	43.862	33.771	33.329		28.82	S
	ATOM	2334		TIP	S	81	57.890	13.106	2.128		40.62	S
	ATOM	2335		TIP	S	82	41.663	34.381	32.043		19.35	S
	ATOM	2336		TIP	S	85	50.974	40.331	19.200		21.14	S
10									-6.556			
10	MOTA	2337		TIP	S	88	47.925	-0.832			24.11	S
	ATOM	2338	OH2		S	90	27.231	28.336	33.481		27.64	S
	ATOM	2339		TIP	S	91	43.651	-7.101	-7.995		24.33	S
	MOTA	2340		TIP	S	92	49.325	4.387	19.370		28.02	S
	ATOM	2341		TIP	S	93	46.231	11.549	33.898		29.40	S
15	MOTA	2342	OH2	TIP	S	94	63.889	24.831	1.168		26.53	S
	MOTA	2343	OH2		s	96	56.396	4.952	-6.749		28.00	S
	ATOM	2344	OH2	TIP	S	98	35.510	27.986	11.558		29.24	S
	MOTA	2345	OH2	TIP	S	100	49.942	24.366	30.265	1.00	31.61	S
	MOTA	2346	OH2	TIP	S	101	56.121	7.113	-8.298	1.00	31.57	S
20	ATOM	2347	OH2	TIP	s	102	58.318	19.957	-8.378	1.00	26.95	S
	ATOM	2348	OH2	TIP	s	103	49.647	22.446	39.624	1.00	40.57	S
	ATOM	2349	OH2	TIP	S	104	45.359	7.052	13.052	1.00	26.27	S
	ATOM	2350	OH2	TIP	s	105	37.150	32.340	32.346	1.00	34.45	S
	ATOM	2351	OH2	TIP	s	107	43.465	40.457	8.240	1.00	40.48	S
25	ATOM	2352	OH2		S	119	36.644	8.257	13.418		30.70	S
	ATOM	2353	OH2	TIP		123	41.912	-8.974	-8.264		26.08	S
	ATOM	2354		TIP		124	62.424	15.800	-7.411		24.08	S
	ATOM	2355	OH2			126	37.266	18.656	-9.097		28.99	s
	ATOM	2356		TIP		127	43.129	26.845	14.606		25.19	s
30	ATOM	2357	OH2	TIP	s	128	36.339	32.639	29.802		29.25	s
50	ATOM	2358	OH2			130	54.051	14.561	26.498		33.93	S
	ATOM	2359		TIP		131	41.805	-4.242	5.492		33.72	S
	ATOM	2360		TIP		133	38.873	25.163	36.697		30.69	S
	ATOM	2360	OH2	TIP	S	134	28.777	8.553	25.307		31.43	S
35		2362		TIP		135	53.672		-12.803		33.45	S
33	ATOM		OH2									
	ATOM	2363	OH2	TIP	S	136	59.892	15.434	11.467		31.39	S
	MOTA	2364		TIP		137	31.040	12.361	35.470		34.07	S
	MOTA	2365	OH2	TIP	S	139	33.489	14.292	-0.598		40.68	S
	MOTA	2366		TIP		140	46.918	8.748	11.662		29.23	S
40	ATOM	2367		TIP	S	141	46.297	-7.287	-9.196		42.20	S
	MOTA	2368	OH2	TIP	S	142	58.193	6.715	-4.685		35.48	S
	MOTA	2369	OH2			143	44.598	4.435	12.503		27.68	S
	MOTA	2370		TIP		144	27.003	5.999	12.450		36.30	S
	MOTA	2371		TIP		145	43.676	32.852	35.735		35.70	S
45	MOTA	2372		TIP	S	146	35.783	18.628	36.452		34.62	S
	MOTA	2373	OH2	TIP	S	147	25.402	4.058	20.638	1.00	45.03	S
	MOTA	2374	OH2	TIP	S	148	45.839	35.853	33.724	1.00	35.47	S
	ATOM	2375	OH2	TIP	S	149	22.176	18.976	16.752	1.00	31.87	S
	MOTA	2376	OH2	TIP	S	150	43.986	33.179	10.162	1.00	37.70	S
50	MOTA	2377	OH2	TIP	s	151	50.653	20.347	42.428	1.00	35.80	S
	MOTA	2378	OH2	TIP	S	152	47.843	24.314	9.506	1.00	31.05	S
	ATOM	2379	OH2	TIP	S	153	44.693	5.273	-14.175	1.00	29.90	S
	MOTA	2380	OH2	TIP	S	155	26.560	36.851	31.684	1.00	49.29	S
	ATOM	2381		TIP		156	46.867		-12.951		29.21	S
55	ATOM	2382		TIP	s	157	30.432	28.741	12.438		37.76	S
	ATOM	2383	OH2			158	41.004	20.553	6.423		39.53	S
	ATOM	2384	OH2	TIP	S	159	49.258	20.069	29.294		33.97	S
	ATOM	2385		TIP			48.082	28.459	16.489		33.10	S
	ATOM	2386		TIP		161	47.448	18.625	27.683		34.87	S

	ATOM	2387	OH2	TIP	s	162	19.687	20.632	23.411	1.00	35.01	S
	ATOM	2388	OH2	TIP			32.402	-1.266	22.443		37.26	S
	ATOM	2389	OH2	TIP	S	164	39.475	33.468	33.237		35.34	S
	ATOM	2390	OH2			165	44.277	18.950	5.162		45.14	s
5	ATOM	2391	OH2				34.797	30.523	10.736		47.55	S
,	ATOM	2392		TIP		167	46.541		-14.949		26.54	S
	ATOM	2392	OH2	TIP	S	168	36.333	16.371	1.539		38.68	S
	ATOM	2394		TIP		169	46.761	38.936	27.403		34.66	S
	MOTA	2395	OH2				24.163	13.264	11.375		41.23	S
10	MOTA	2396		TIP		171	48.459	15.018	31.951		38.11	S
	MOTA	2397	OH2	TIP	S	172	34.261	23.193	40.004		48.96	S
	ATOM	2398	OH2	TIP			45.924	-0.026	13.224		39.55	S
	ATOM	2399		TIP	S	175	41.384	37.389	32.543	1.00	40.74	S
	MOTA	2400	OH2	TIP	S	177	49.394	35.312	27.150	1.00	44.33	S
15	MOTA	2401	OH2	TIP	s	178	29.066	29.942	34.359	1.00	41.46	S
	ATOM	2402	OH2	TIP	s	180	49.354	19.467	7.273	1.00	34.56	S
	MOTA	2403	OH2	TIP	S	181	25.298	17.029	31.863	1.00	47.74	S
	ATOM	2404	OH2	TIP	s	182	37.071	25.027	4.669	1.00	43.87	S
	ATOM	2405	OH2	TIP	s	183	22.581	7.487	18.691	1.00	41.75	S
20	ATOM	2406	OH2	TIP	S	184	32.269	7.011	-1.891		48.84	S
	ATOM	2407	OH2	TIP	S	185	48.234	0.494	6.833		48.16	S
	ATOM	2408	OH2	TIP			20.008	14.658	19.211		45.27	S
	ATOM	2409		TIP		188	49.341	22.698	42.272		42.20	s
	ATOM	2410	OH2	TIP			61.292	18.260	-8.097		45.21	S
25	ATOM	2411	OH2				28.152	10.606	2.819		40.38	S
23	ATOM	2411	OH2	TIP			25.626	12.619	23.191		34.27	S
	ATOM	2412		TIP		193					46.54	S
							59.876	11.603	1.216			S
	ATOM	2414	OH2			194	57.592		-10.646		45.82	
	MOTA	2415	OH2			195	31.509	36.649	21.499		38.73	S
30	MOTA	2416	OH2	TIP	S	197	50.270	-1.543	-6.136		42.66	S
	MOTA	2417	OH2	TIP		198	24.467	8.729	13.088		42.78	S
	ATOM	2418		TIP		199	38.098	8.699	25.759		32.80	S
	MOTA	2419		TIP			57.831		-13.255		45.31	S
	ATOM	2420	OH2	TIP	S	201	23.888	22.328	30.524		37.12	S
35	ATOM	2421	OH2	TIP	S	202	47.691	26.068	37.666	1.00	37.92	S
	MOTA	2422	OH2	TIP	S	203	38.653	7.070	29.307	1.00	50.54	S
	ATOM	2423	OH2	TIP	S	206	44.424	27.583	2.092	1.00	53.50	S
	ATOM	2424	OH2	TIP	S	212	22.258	2.296	17.948	1.00	47.38	S
	ATOM	2425	OH2	TIP	S	214	19.843	17.943	23.303	1.00	30.36	S
40	ATOM	2426	OH2	TIP	S	216	27.647	11.344	24.681	1.00	31.32	S
	ATOM	2427	OH2	TIP	s	217	37.953	7.817	-9.284	1.00	45.97	S
	MOTA	2428	OH2	TIP	S	218	33.845	34.040	12.124	1.00	38.11	S
	ATOM	2429	OH2	TIP	s	219	58.484	15.269	13.717		38.26	S
	ATOM	2430	OH2	TIP	s	220	48.526	40.920	26.583		35.23	S
45	ATOM	2431	OH2	TIP		222	52.094	21.184	38.122	1.00	29.86	S
	ATOM	2432	OH2	TIP		223	36.889	5.881	3.281		37.63	s
	ATOM	2433	OH2				47.642		-10.684		34.89	S
	ATOM	2434		TIP		226	47.284	2.916	19.133		34.10	S
	ATOM	2435		TIP			42.468		-15.039		37.98	s
50	ATOM	2436		TIP		228	19.169	22.832	21.831		41.57	s
50	ATOM	2436	OH2				57.592	12.689	14.880		50.22	S
				TIP								S
	ATOM	2438	OH2			232	27.102	9.176	5.655		40.57	
	MOTA	2439	OH2	TIP			58.618		-11.925		50.71	S
	ATOM	2440		TIP		234	22.822	25.342	19.945		34.93	S
55	MOTA	2441	OH2		S	236	24.831	32.218	28.901		37.69	S
	MOTA	2442	OH2			237	20.045	10.774	16.992		39.57	S
	MOTA	2443	OH2	TIP	S	238	58.019	19.850	15.679		41.42	S
	MOTA	2444		TIP			19.490	20.949	26.114		34.55	S
	ATOM	2445	OH2	TIP	S	240	61.187	26.377	7.346	1.00	39.68	S

	ATOM	2446	OH2	TIP	s	241	33.680	38.342	19.389	1.00	48.93	S
	ATOM	2447	OH2				51.539	31.612	10.881		55.65	S
	ATOM	2448		TIP		244	25.872	14.431	30.404		46.69	S
	ATOM	2449		TIP		248	37.332	5.849	9.544		43.81	S
5	ATOM	2450		TIP		250	39.087	-1.293	-9.655		42.96	S
-	MOTA	2451		TIP		258	23.938	30.000	30.010		38.89	S
	ATOM	2452		TIP		259	24.949	29.749	32.578		40.17	S
	ATOM	2453		TIP		260	32.111	17.986	1.918		48.36	S
	ATOM	2454		TIP		266	21.404	12.876	25.603		57.17	S
10		2454		TIP					12.550			
10	MOTA					269	35.425	36.767			30.70	S
	ATOM	2456	OH2	TIP	S	270	52.438	25.529	30.131		44.85	S
	ATOM	2457		TIP		271	53.299	20.156	36.003		37.15	S
	MOTA	2458		TIP		272	50.914	6.919	23.723		43.29	S
	ATOM	2459		TIP		274	31.578	30.795	11.014		50.15	S
15	MOTA	2460	OH2	TIP	s	275	26.341	7.243	22.447		39.40	S
	MOTA	2461	OH2	TIP	S	276	60.392	18.195	10.235		37.91	S
	ATOM	2462	OH2	TIP	S	277	47.355		-10.821	1.00	48.18	S
	MOTA	2463	OH2	TIP	S	279	41.304	6.175	-16.647	1.00	38.12	S
	ATOM	2464	OH2	TIP	s	282	33.299	21.620	37.881	1.00	46.29	S
20	ATOM	2465	OH2	TIP	s	283	56.469	26.112	-8.575	1.00	43.71	S
	ATOM	2466	OH2	TIP	S	287	48.382	26.573	7.246	1.00	41.43	S
	MOTA	2467	OH2	TIP	S	288	56.240	7.245	-11.331	1.00	41.79	S
	ATOM	2468	OH2	TIP	s	290	49.060	14.978	28.166	1.00	37.03	S
	ATOM	2469	OH2	TIP	s	291	37.095	44.270	26.442	1.00	45.08	S
25	ATOM	2470	OH2	TIP	s	292	47.814	-0.384	-13.299	1.00	48.60	S
	ATOM	2471	OH2	TIP	s	297	58.081	2.784	-7.841	1.00	41.89	S
	ATOM	2472	OH2	TIP	S	298	36.447	45.321	18.644	1.00	54.91	S
	ATOM	2473		TIP			49.029	23.328	1.767		30.55	S
	ATOM	2474		TIP		301	24.375	13.771	8.634		48.47	s
30	ATOM	2475	OH2	TIP	s	303	47.904	36.798	28.653		35.76	s
50	ATOM	2476		TIP		305	51.156	40.821	27.172		43.59	s
	ATOM	2477		TIP		306	32,943	28.917	35.227		42.60	S
	ATOM	2478		TIP		307	58.462	28.373	6.251		46.15	S
	ATOM	2479		TIP		308	41.964	30.940	36.712		48.26	S
35	ATOM	2480	OH2	TIP			51.176	-1.922	-3.336		50.61	S
33	ATOM	2481		TIP			21.319	36.868	23.805		36.97	S
	ATOM	2482		TIP			48.880	32.620	27.617		44.40	S
	MOTA	2483		TIP			61.880	19.473	11.767		45.49	S
40	ATOM	2484		TIP			52.770	21.424	26.815		24.43	S
40	ATOM	2485		TIP			35.373	29.094	36.197		35.97	S
	ATOM	2486		TIP			40.815	-6.636	4.389		43.15	S
	ATOM	2487		TIP			44.953	1.286	11.272		49.45	S
	ATOM	2488		TIP			21.004	16.168	27.009		48.51	S
	ATOM	2489		TIP			47.094	41.786	9.243		50.10	S
45	ATOM	2490		TIP			32.479	2.978	14.158		49.47	S
	MOTA	2491			G	1	48.557		-12.279		40.72	G
	MOTA	2492		GLC		1	48.836		-11.097		38.05	G
	MOTA	2493		GLC		1	49.266		-11.476		38.09	G
	MOTA	2494		GLC		1	49.559		-10.292		33.99	G
50	MOTA	2495		GLC		1	48.150		-12.257		37.32	G
	ATOM	2496		GLC		1	48.574		-12.604		36.74	G
	MOTA	2497		GLC		2	40.114	-6.634	-6.562		33.52	G
	MOTA	2498	C11	GLC	G	2	38.967	-6.592	-7.404	1.00	31.05	G
	ATOM	2499	C13	GLC	G	2	37.712	-6.417	-6.552	1.00	31.56	G
55	MOTA	2500	014	GLC	G	2	36.554	-6.406	-7.389	1.00	30.70	G
	MOTA	2501	C15	GLC	G	2	37.792	-5.109	-5.761	1.00	30.03	G
	MOTA	2502	016	GLC	G	2	36.609	-4.961	-4.975	1.00	29.66	G
	MOTA	2503	012	GLC	G	3	44.030	8.243	-13.470	1.00	37.90	G
	ATOM	2504	C11	GLC	G	3	43.950	9.648	-13.690	1.00	38.47	G

	ATOM	2505	C13	GLC	G	3		12.747	9.974	-14.579	1.00	39.52	G
	MOTA	2506	014	GLC	G	3		11.551	9.526	-13.942	1.00	39.39	G
	ATOM	2507		GLC	G	3		12.878		-15.934		41.43	G
	ATOM	2508		GLC	G	3		11.736		-16.731		40.78	G
5				GLC	G					2.289		45.25	
3	MOTA	2509				5		10.556	1.005				G
	MOTA	2510		GLC	G	5		10.966	2.332	1.960		40.56	G
	MOTA	2511		GLC	G	5		10.187	3.327	2.814		40.36	G
	MOTA	2512			G	5		38.791	3.169	2.572		40.71	G
	MOTA	2513	C15	GLC	G	5	4	10.619	4.751	2.464	1.00	40.04	G
10	MOTA	2514	016	GLC	G	5		39.885	5.681	3.256	1.00	36.89	G
	MOTA	2515	012	GLC	G	6		36.951	22,702	40.046	1.00	63.04	G
	MOTA	2516	C11	GLC	G	6		37.592	21.583	39.422	1.00	62.46	G
	ATOM	2517		GLC		6		38.104	21.978	38.030		61.14	G
	ATOM	2518		GLC		6		39.034	23.054	38.168		61.72	G
15	MOTA	2519		GLC		6		36.948	22.429	37.126		60.51	G
15	ATOM	2520			G	6		35.992	21.372	36.960		58.61	G
	MOTA	2521			G	7		37.316	0.281	14.299		73.45	G
	MOTA	2522			G	7		37.655	-0.758	15.222		72.78	G
	MOTA	2523		GLC		7		36.592	-1.856	15.157		72.98	G
20	MOTA	2524			G	7		35.320	-1.299	15.498		73.88	G
	MOTA	2525			G	7		36.924	-2.989	16.134		73.66	G
	MOTA	2526	016	GLC	G	7		36.972	-2.493	17.478	1.00	75.38	G
	MOTA	2527	012	GLC	G	8		51.921	21.898	5.908	1.00	62.51	G
	MOTA	2528	C11	GLC	G	8		52.447	20.871	5.063	1.00	63.42	G
25	MOTA	2529	C13	GLC	G	8		51.476	20.597	3.908	1.00	64.28	G
	MOTA	2530	014	GLC	G	8		51.297	21.794	3.150	1.00	66.28	G
	MOTA	2531		GLC	G	8		50.121	20.137	4.448		64.49	G
	ATOM	2532		GLC	G	8		19.233	19.886	3.357		64.01	G
	MOTA	2533			G	10		36.044	37.499	29.523		56.89	G
30	ATOM	2534		GLC	G	10		35.164	36.645	30.259		56.97	G
50	ATOM	2535		GLC	G	10		33.849	36.489	29.494		56.11	G
				GLC	G								
	MOTA	2536				10		33.248	37.772	29.308		56.44	G
	MOTA	2537			G	10		32.900	35.580	30.277		55.84	G
	MOTA	2538			G	10		31.674	35.442	29.557		55.39	G
35	MOTA	2539		ATP	N	1		16.280	25.658	5.170		51.49	N
	MOTA	2540	PG	ATP	N	1		16.464	25.053	3.691		52.22	N
	MOTA	2541		ATP	N	1		17.406	23.911	3.763		51.41	N
	MOTA	2542	02G	ATP	N	1	4	16.794	26.182	2.784	1.00	52.07	N
	MOTA	2543	03B	ATP	N	1		14.976	24.513	3.344	1.00	51.01	N
40	MOTA	2544	PB	ATP	N	1	4	14.560	22.969	3.605	1.00	50.20	N
	MOTA	2545	01B	ATP	N	1		13.083	22.898	3.669	1.00	49.41	N
	MOTA	2546	02B	ATP	N	1		15.345	22.474	4.766	1.00	50.34	N
	MOTA	2547	03A	ATP	N	1		15.070	22,231	2.255	1.00	47.77	N
	ATOM	2548	PA	ATP		1		15.075	20.613	2.121		42.84	N
45	ATOM	2549		ATP		1		15.547	20.291	0.754		43.81	N
75	ATOM	2550		ATP		1		15.807	20.035	3.270		45.03	N
	ATOM	2551		ATP		1		13.516	20.033	2.245		41.73	N
					N								
	MOTA	2552		ATP	N	1		12.528	20.925	1.489		37.57	N
	MOTA	2553		ATP	N	1		11.127	20.379	1.776		39.45	N
50	MOTA	2554		ATP	N	1		10.907	19.024	1.279		37.72	N
	MOTA	2555	C3*		N	1		10.777	20.321	3.251		38.48	N
	MOTA	2556		ATP	N	1		10.360	21.615	3.697		40.42	N
	MOTA	2557	C2*	ATP	N	1		39.608	19.374	3.270	1.00	37.58	N
	MOTA	2558	02*	ATP	N	1		38.410	20.076	2.924	1.00	35.98	N
55	MOTA	2559	C1*	ATP	N	1		39.939	18.346	2.173		35.55	N
	ATOM	2560	N9	ATP	N	1		10.628	17.156	2.747	1.00		N
	ATOM	2561	C8	ATP		î		11.864	17.126	3.274		30.49	N
	ATOM	2562	N7	ATP		1		12.143	15.877	3.667		29.75	N
	ATOM	2563	C5	ATP		1		11.088	15.118	3.390		27.49	N
	111011	2000		I I	-4	-	-		10.110	5.550	1.00		14

	MOTA	2564	C4	ATP	N	1	40.125	15.925	2.810	1.00 30.02	N
	MOTA	2565	N3	ATP	N	1	38.937	15.389	2.431	1.00 27.11	N
	MOTA	2566	C2	ATP	N	1	38.679	14.085	2.615	1.00 25.62	N
	MOTA	2567	N1	ATP	N	1	39.597	13.283	3.175	1.00 21.76	N
5	ATOM	2568	C6	ATP	N	1	40.800	13.768	3.571	1.00 23.90	N
	MOTA	2569	N6	ATP	N	1	41.698	12.964	4.127	1.00 21.94	N
	MOTA	2570	S	SO4	I	1	58.680	8.493	-0.639	1.00 56.05	I
	MOTA	2571	01	SO4	I	1	57.956	7.875	0.483	1.00 58.83	I
	MOTA	2572	02	SO4	Ι	1	57.886	9.607	-1.188	1.00 57.04	I
10	MOTA	2573	03	SO4	Ι	1	58.906	7.478	-1.683	1.00 57.47	I
	MOTA	2574	04			1	59.976	9.008	-0.156	1.00 57.51	I
	MOTA	2575	S	SO4	Ι	2	39.339	4.855	7.057	1.00 84.24	I
	MOTA	2576	01	SO4	I	2	39.390	6.175	7.711	1.00 85.02	I
	MOTA	2577	02	SO4		2	40.101	4.897	5.797	1.00 84.75	I
15	MOTA	2578	03			2	37.936	4.506	6.766	1.00 84.94	I
	MOTA	2579	04	SO4	Ι	2	39.931	3.842	7.954	1.00 84.44	I
	MOTA	2580	S	SO4	Ι	3	38.987	-2.256	3.310	1.00 58.58	I
	MOTA	2581	01			3	37.734	-1.675	3.827	1.00 59.11	I
	MOTA	2582	02		Ι	3	39.460	-1.454	2.172	1.00 59.91	I
20	MOTA	2583	03	SO4		3	38.743	-3.640	2.866	1.00 60.97	I
	MOTA	2584	04	SO4	Ι	3	40.014	-2.260	4.369	1.00 59.58	I
	MOTA	2585	S		I	4	34.397	5.289	30.981	1.00 64.34	I
	MOTA	2586	01		Ι	4	33.627	6.528	30.742	1.00 60.43	I
	MOTA	2587	02			4	34.337	4.427	29.782	1.00 60.11	I
25	MOTA	2588	03	SO4	Ι	4	33.816	4.572	32.133	1.00 64.39	I
	MOTA	2589	04	SO4	Ι	4	35.806	5.626	31.277	1.00 63.55	I
	MOTA	2590	S		Ι	5	55.074	-6.984	-3.711	1.00 75.40	I
	MOTA	2591	01		I	5	54.657	-7.518	-2.399	1.00 74.66	I
	MOTA	2592	02		Ι	5	54.209	-5.845	-4.065	1.00 74.96	I
30	MOTA	2593	03	SO4	Ι	5	54.950	-8.034	-4.742	1.00 74.22	I
	MOTA	2594	04	SO4		5	56.477	-6.532	-3.633	1.00 75.15	I
	MOTA	2595	02	PO4		100	57.362	24.998	13.149	1.00 66.76	P
	MOTA	2596	03	PO4		100	59.399	26.166	13.761	1.00 66.89	P
	MOTA	2597	04	PO4		100	57.761	25.606	15.462	1.00 67.43	P
35	MOTA	2598	01	PO4		100	57.264	27.325	13.818	1.00 65.91	P
	MOTA	2599	P	PO4	Ρ	100	57.947	26.025	14.048	1.00 66.69	P
	END										

Example 5: PDK1 fragments

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We produced constructs for expression of different forms of PDK1 in bacteria. The constructs were either in TRC vectors, pET-15b vector and pGEX expression vector to enable the expression of GST fused N-terminally to PDK1. PDK1 expressed from pGEX 51-556 (ie residues 51 to 556 of PDK1) was found to be highly degraded.

PDK1 protein was also expressed with N-terminal His tags from vector TRC comprising PDK1 sequences 51-556, 51-404 and 1-360, or pET15b 51-404 and tested for expression levels and activity. The expression was generally low, around 0.2 mg/L culture. The specific activity was lower than the His-tagged 51-556 protein purified from baculovirus cells. In the case of PDK1 51-404 expressed from pET-15b construct the level of expression turned out to be very variable. This was probably due to instability of the plasmid since we produced evidence that after a growth of 0.2 units of absorbance, (as measured in a spectrophotometer at 600 nm wavelength) the cells growing faster in the culture were actually not harbouring the plasmid with ampiciline resistance. The instability of the plasmid can be due to toxicity produced by basal expression of PDK1. Although production in bacteria was the theoretical best expression system to avoid heterogeneity due to the different extent of phosphorylation of the different phosphorylation sites in hPDK1, it was found that the protein was either degraded, expressed to low levels, had 5 times less specific activity, or was possibly toxic.

The His-tagged purified PDK1 51-556 protein obtained from baculovirus expression system was homogeneous as depicted by the appearance of one band after by SDS-PAGE analysis of a sample.

Nevertheless, the analysis after isoelectric focussing revealed a large smear of protein covering several units of pH. This analysis suggested that the protein was not homogeneous in terms of its isoelectric point, possibly due to the number of phosphorylation sites which were not homogeneously phosphorylated. This protein did not crystallise.

We purified to homogeneity a truncated His-Myc tagged PDK1 (51-404) which lacks the N-terminal 50 residues and the C-terminal 152 residues which include the PH domain. This protein, produced by a baculovirus expression system, had similar characteristics to the full length wild type PDK1 in terms of its activity towards the peptide substrate T308tide, its activation by the peptide PIFtide, and the binding to PIFtide (as analysed by BiaCore). The purified protein was screened for crystallisation conditions using Hampton Research kits (144 different conditions). Crystallisation conditions were screened with two concentrations of PDK1, in the presence or absence of PIFtide, Staurosporine, at 20°C and in the presence of PIFtide at 4°C. No protein crystals were observed after 6 months, suggesting that this construct was not suitable for forming crystals although all other characteristics were similar to wild type protein.

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The His-Myc PDK1 51-404 purified protein was also subjected to protease treatments in order to obtain a protease-insensitive molecule for increasing the chances of obtaining a shorter, stable variant of PDK1. Different protease treatments were tested. Treatment with Glu-C produced a polypeptide of approximately 38 KDa which was stable. This PDK1 protein was active and lacked the His-tag and part of the Myc-tag, and possibly part of the C-terminal residues. This protein was also set up for crystallography screenings. Some crystals were obtained using this preparation after 4 months, but they were not followed up.

A protein kinase corresponding to residues PDk1 51-387 was also produced, in an identical vector to that used to produce the protein PDK1 51-359. Interestingly, this protein was similar to wild type and PDK1 51-404, but had extreme problems for concentration using conventional methods. The protein could not be concentrated further than 2.5 mg/ml, and no crystals were obtained using this construct.

The PDK1 protein that finally crystallised is lacking the first 50 aminoacids and was constructed to end at position 359. This protein was stable in the absence of the PH domain and aminoacids that in hPDK1 link the catalytic domain with the PH domain. The construct PDK1 51-359 was also short enough that no other described phosphorylation sites besides activation loop phosphorylation site 241 were present.

5 Example 6: Structural basis for UCN-01 specificity and PDK1 inhibition

The staurosporine derivative UCN-01 (7- hydroxyl staurosporine) has been reported to be a potent inhibitor for PDK1 and is currently in clinical trials for the treatment of cancer. Here we report the crystal structures of staurosporine and UCN-01 in complex with the kinase domain of PDK1. We show that although staurosporine and UCN-01 interact with the PDK1 active site in an overall similar manner, the UCN-01 7-hydroxylgroup, which is not present on staurosporine, generates direct and water-mediated hydrogen bonds with active site residues. Inhibition data from UCN-01 tested against a panel of 29 different kinases show a different pattern of inhibition compared to staurosporine. We discuss how these differences in inhibition could be attributed to specific interactions with the additional 7-hydroxyl-group as well as by the size of the 7-hydroxyl-binding pocket. This information could lead to opportunities for structure-based optimisation of PDK1 inhibitors.

Insulin and growth factor signalling is mediated by the activation of a lipid kinase, phosphatidylinositol-3-kinase (PI3K), which produces the second molecule phosphatidylinositol(3,4,5)trisphosphate messenger (PtdIns(3,4,5)P) [1]. Upon generation of PtdIns(3,4,5)P, 3-Phosphoinositide Dependent protein Kinase-1 (PDK1) and protein kinase B (PKB, also known as Akt) are co-localised at the plasma membrane through interaction of their Pleckstrin Homology (PH) domains with PtdIns(3,4,5)P [2, 3]. PDK1 activates PKB by phosphorylation of its T-loop (Thr308 in PKB) [4, 5]. PDK1 also activates other protein kinases related to PKB, including isoforms of p70 ribosomal S6 kinase (S6K) [6], serum and glucocorticoid responsive kinases (SGK) [7] and p90 ribosomal S6 kinase (Rsk) [8]. These kinases lack PH domains and do not bind PtdIns(3,4,5)P3, and are thought to be activated by a different mechanism, in which the substrates require a priming phosphorylation in a conserved hydrophobic motif (HM) at their Cterminus (reviewed in [9]). This phosphorylation creates a docking motif that specifically interacts with a pocket on the N-terminal lobe of the PDK1 kinase domain (termed PDK1 interacting fragment (PIF) pocket) [10, 11] bringing PDK1 together with its substrate and enabling PDK1 to phosphorylate these kinases in their T-loop, thereby activating them. A significant number of human cancers possess elevated PtdIns(3,4,5)Plevels due to mutations in a number of genes that regulate the production and degradation of this 3-phosphoinositide. One of the most frequently found mutations occurs in the PtdIns(3,4,5)P 3-phosphatase (PTEN) resulting in constitutive activation of PKB and S6K, which are thought to be major 25 contributors to the proliferation and the survival of such tumour cells [12]. Thus, inhibitors of PDK1 have the potential to act as anti-cancer agents as they would be expected to suppress activation of S6K and PKB and inhibit cell growth and induce apoptosis of cancer cells that possess elevated levels of PtdIns(3,4,5)P. 30

PDK1 consists of an N-terminal kinase domain and a C-terminal PHdomain [13]. The structure of the PDK1 kinase domain has been solved (see the preceding Examples and [11]) and leads to a definition of the residues lining the ATP binding site and an understanding of the PDK1 activation mechanism. The PIFbinding pocket could be identified, together with a specific pocket for the phosphorylated Ser/Thr residue on the HM of substrate kinases. Staurosporine, a natural product ATP-competitive inhibitor, inhibits many kinases in the low nM range [14], and therefore displays a high cytotoxicity [15]. UCN-01 (7-hydroxyl staurosporine) is a derivative with an additional hydroxyl group on the lactam ring (Fig. 1). It was originally described as a PKC-selective inhibitor isolated from Streptomyces sp. cultures [16], although further studies showed it to be more non-specific [14, 17]. UCN-01 potently inhibits the growth and induces apoptosis of many cancer cells and these effects are thought to be unrelated to PKC inhibition [18, 19]. Due to its anti-tumour activity in vivo and in vitro, UCN-01 is currently undergoing clinical trials with positive effects being reported in the phase 1 studies (reviewed in [19]). Recent reports suggested the cell cycle checkpoint kinase Chk1 [20] and PDK1 [21] may be key targets of UCN-01 in inhibiting the growth of cancer cells, as both kinases are inhibited by UCN-01 in the low nM range.

Here we report the structures of the PDK1 kinase domain in complex with staurosporine and UCN-01, demonstrating the presence of a pocket that accommodates the 7-hydroxyl group of UCN-01. Specificity tests against a panel of 29 kinases shows that although both staurosporine and UCN-01 are relatively non-specific inhibitors, the fingerprint analysis of UCN-01 inhibition with a panel of protein kinases is significantly different from that of staurosporine. We also perform analysis of residues predicted to line the UCN-01 hydroxyl pocket on a number or protein kinases, and propose a

general model that could account for the different sensitivity of protein kinases for staurosporine and UCN-01.

Methods

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5 Expression, purification and crystallisation

Human PDK1 (residues 51-359) was expressed using a baculovirus mediated infection of the SF21 insect cell line and purified as described in the preceding examples and [11] with the following differences: After elution of the His-tagged protein from the Ni-NTA-agarose beads with 200 mM imidazole, the protein was dialysed against 250 mM NaCl, 25 mM Tris pH 7.5, 1 mM DTT for 3 hours at 4°C. Proteolysis with GST-tagged PreScission protease was performed overnight at 4 °C.

For crystals of the PDK1-UCN-01 complex, 100 µl of PDK1 at a concentration of 6.6 mg/ml was mixed with 30 µl UCN-01 (5.3 mM in 50 % ethanol) and incubated on ice for 2 hours. The protein was crystallized using sitting drop vapour diffusion. 1.25 µl of protein solution was mixed with 0.25 µl cobaltous chloride hexahydrate (0.1 M) and 1 µl mother liquor, consisting of 2.1 M ammonium sulphate, 0.1 M Tris-HCl pH 8.5. Hexagonal, rod-shaped crystals grew at 20 °C and reached a maximum size of 0.05 x 0.05 x 0.3 mm after 7 days. After soaking for 3 seconds in a cryo-protection solution (2.1 M ammonium sulphate, 0.1 M Tris-HCl pH 7.2, 25 % glycerol) crystals were frozen in a stream of cold nitrogen.

25 PDK1 in complex with staurosporine was crystallized using the hanging drop technique. Drops consisted of 1µ1 PDK1 at 7.6 mg/ml, 1 µ1 mother liquor (2.1 M ammonium sulphate, 0.1 M Tris- HCl pH 7.2) and 0.25 µ1 staurosporine (10 mM in DMSO). Hexagonal shaped crystals suitable for

data collection appeared after 6 weeks at 20 C. Crystals were soaked in 1.7 M ammonium sulphate, 0.1 M Tris-HCl pH 7.2, 15% glycerol and frozen in a stream of cold nitrogen.

Data collection, structure solution and refinement

Data on the PDK1-staurosporine and PDK1-UCN-01 complexes were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH4. The temperature of the crystals was maintained at 100 K using a nitrogen cryostream. Data were processed using the HKL package [22] with final statistics shown in Table 3. The structures were solved by rigid body refinement with CNS [23] using the previously determined PDK1 structure (See previous Examples; PDB code 1H1W) [11] as a starting model which resulted in an initial R-factor of 0.306 (R_{free} = 0.284) for PDK1-staurosporine and 0.299 (R_{free} = 0.311) for PDK1-UCN-01. Model building with O [24] and iterative refinement in CNS, including solvent molecules and the T-loop phosphorylation site, resulted in final R-factors as shown in Table 3. The ATP binding site showed well-defined density in the unbiased $|F_o|-|F_c|$, ϕ_{calc} maps for all atoms of staurosporine and UCN-01, including the 7-hydroxyl group (Fig. 8). CNS topologies and coordinates for the inhibitors were generated with PRODRG [25]. No electron density could be observed for residues 51-72 (N-terminus), residues 231-239 (T-loop) and residue 359 (C-terminus) in the PDK1-UCN-01 complex. Residues 51-71 (N-terminus) and 233-238 (Tloop) were disordered in the PDK1-staurosporine complex.

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Determination of inhibition and specificity

Protein kinase assays: PDK1 was assayed for 10 min at 30 °C in a 50 μl assay mixture in 50 mM Tris pH 7.5, 0.1 mM EGTA, 0.1% 2-

mercaptoethanol, containing 100 μ M PDK1tide substrate peptide (KTFCGTPEYLAPEVRREPRILSEEEQEMFRDFDYIADWC) (SEQ ID NO:112), 10 mM magnesium acetate, 100 μ M [γ -³²P]ATP (200 cpm/pmole) as described previously [10]. Other protein kinases employed in Table 5, were assayed as described previously [17, 26].

Results & Discussion

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Structures of the staurosporine and UCN-01 complexes

PDK1 (residues 51-359) was co-crystallized with staurosporine and UCN-01, and synchrotron diffraction data on a thin hexagonal needle were collected to 2.3 Å and 2.5 Å resolution, respectively.

In the unbiased $|F_o|$ - $|F_c|$, ϕ_{calc} maps well defined (>3.0 σ) density could be observed in the ATP binding site of the kinase, covering all staurosporine/UCN-01 atoms including the 7-hydroxyl group (Fig. 8). After initial rounds of protein model building and inclusion of water molecules, the inhibitor molecules were built and refined with full occupancy to average B-factor of 18.5 Ų (staurosporine) and 17.3 Ų(UCN-01). Further refinement resulted in a final PDK1-staurosporine model with R = 0.218 (R_{free} = 0.255) and a final PDK1-UCN-01 model with R = 0.184 (R_{free} = 0.257), both with good stereochemistry (Table 3).

The staurosporine molecule is located in the ATP-binding site (which lies between the N-terminal and C-terminal lobes of kinases [27, 28]), at the same position described for the inhibitor in complex with the closely related (38 % sequence identity) protein kinase A (PKA, [29], PDB code 1STC) (Fig. 8). Hydrophobic residues on both sides of the ATP binding cleft sandwich the heterocyclic moiety of staurosporine, namely Leu88, Val96, Ala109, Leu98 (small lobe) and Thr222, Leu212 of the larger lobe (Fig. 1).

Similar to the PKA-staurosporine complex, the lactam group mimics the interactions of the adenine base in ATP with the protein backbone, where 2 conserved hydrogen bonds are formed between the lactam-nitrogen N6 in staurosporine (nomenclature according to [30]) and the backbone-oxygen of Ser160, and the lactam-oxygen at the C5 position and the backbone-nitrogen of Ala162 (Table 4). An additional hydrogen bond is mimicked in the staurosporine sugar-moiety, where the methyl-amino group contacts oxygen O 2 of Glu166, similar to the hydrogen bond with the ribose in the PDK1-ATP complex [11], and also the backbone carbonyl of Glu209 (Table 4).

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The UCN-01 molecule occupies the same position in the ATP binding site as staurosporine (maximum atomic shift = 0.35 Å) (Fig. 9). The same hydrophobic interactions are made to the heterocyclic moiety in the PDK1staurosporine complex. Hydrogen bonding interactions to the heterocycle and the sugar moiety are also conserved, with similar geometry (Table 4). However, the 7-hydroxyl group of UCN-01 forms several novel hydrogen bonds (Fig. 9, Table 4). It hydrogen bonds directly to Oy 1 of Thr222 (Fig. 9, Table 4). In addition, an ordered water molecule (B-factor = 24.0 Å²) is found in a position where it contacts the 7-hydroxyl (distance = 3.0 Å, Table 4) and the oxygen O_E1 of Gln220 (distance = 2.5 Å) the side chain of which is shifted towards the ligand (1.5 Å for Cδ, rotation of 82° around γ₁) compared to the PDK1-STO complex. However, the water molecule is buried in a predominantly hydrophobic pocket, lined by Val143, Leu212 and Cy2 of Thr222 (Fig. 9). Val143 also changes its position compared to the PDK1-staurosporine complex (Fig. 9), moving further towards the back of the pocket (shift of 0.7 °A for the Cα carbon, and a rotation of 100° around χ_1) and displaces an ordered water molecule present in the PDK1staurosporine complex (Fig. 9), and also observed in other kinasestaurosporine complexes [31, 30]. These changes result in more space to accommodate the bulky 7-hydroxyl group on UCN-01 as indicated by a 6 °A³ increase in ligand volume (calculated with VOIDOO [32]).

Comparison with Chk1-UCN-01

High resolution data for the Chk1 kinase bound to staurosporine and UCN-01 is available (PDB code 1NVQ [30]). In Chk1, Ser147, the equivalent of Thr222 in PDK1, also hydrogen bonds the UCN-01 7-OH directly. In addition, a water mediated network of hydrogen bonds to UCN-01 is observed. However, in Chk1 the water molecule that hydrogen bonds UCN-01 occupies a different position (shifted 5.2 Å compared to the PDK1-UCN-01 complex). Chk1 appears to have a more extended hydrophilic cavity, as there are 2 additional buried water molecules present also in the Chk1-staurosporine complex. The corresponding residue to Gln220 in PDK1 is a Lys (Lys145) in Chk1, which does not interact with the ligand but points away from it.

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UCN-01 inhibition and specificity

PDK1 inhibition by UCN-01 and staurosporine was measured using kinase assays with P³²-labelled ATP. PDK1 is inhibited by UCN-01 with an IC₅₀ value of 5 nM, and by staurosporine with an IC₅₀ of 6.5 nM. As a measure for overall specificity of UCN-01 and staurosporine, the effect of these inhibitors was tested against a panel of 29 protein kinases as described previously [17, 26]. The results are shown in Table 5 as percentage of control activity. These data further confirm that UCN-01 and staurosporine are aspecific inhibitors. UCN-01 at 1 μM concentration reduces the activity of nine kinases in the panel to less than 10%, and of ten others to below 60% of control activity. Staurosporine at 1 μM will inhibit twelve kinases to less than 10% control activity, and another ten to below 60%. Interestingly, however, several of the protein kinases were differentially inhibited by

staurosporine and UCN-01 (Table 5). In an attempt to understand these differences the panel of kinases was divided in four distinct classes: (a) similar inhibition, (b) stronger inhibition by staurosporine than by UCN-01, (c) stronger inhibition by UCN-01 than by staurosporine, and (d) no inhibition (Table 5). As the additional 7-hydroxyl group is the only difference in the ligand molecules (Fig. 8), and staurosporine and UCN-01 occupy the same position with similar interactions in the binding site (Fig.9), the residues contacting the extra hydroxyl group were identified for PDK1 and extracted from a sequence alignment of all protein kinases used in the panel (Table 5). A structure-based sequence alignment of known kinase structures was obtained from [33], which was used to validate the sequence-based sequence alignment (Table 5). The nature of the side chains lining the hydroxyl-pocket could provide a partial explanation for the relative difference between UCN-01 and staurosporine inhibition. Two trends can be observed. For the kinases that are inhibited by UCN-01, there appears to be a preference for a side chain capable of hydrogen bonding the 7-hydroxyl in the hydroxyl-pocket. This is in agreement with the presence of a Thr/Ser residue that hydrogen bonds the 7-hydroxyl in the structures of PDK1 (Thr222) and Chk1 (Ser147) bound to UCN-01. Seven out of ten kinases that are hit equally by staurosporine and UCN-01 (group (a)) appear to have a potential hydrogen bonding residue (Table 5). The kinases that are more potently inhibited by UCN-01 than by staurosporine (group (c)) contain a Thr at the Thr222 equivalent position (Table 5). Five out of nine kinases that are inhibited more potently by staurosporine than by UCN-01 (group (b)) lack a potential hydrogen binding partner in the 7-hydroxylpocket (Table 5).

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A second trend which appears to determine specificity is the size of the residues lining the hydroxyl-pocket. If the predicted total volume of the residues (calculated with the BL- set of side chain volumes [34]) at the

positions indicated in Table 5 is set against the activity in the presence of UCN-01, a correlation coefficient of 0.6 is obtained. This suggests that despite inaccuracies in this approach, such as the absence of structural information on precise side chain conformation and water molecules, a weak correlation between predicted hydroxyl pocket volume and UCN-01 inhibition exists. For instance, PKA contains a possible hydrogen bonding partner for UCN-01 (Thr183), but Met134 in the centre of the hydroxyl pocket may leave no space for the extra hydroxyl group (Table 5). A similar arrangement of residues can be observed for MAPKAP-K2 (Table 5). This size dependency may also play a role for the protein kinases neither hit by staurosporine nor UCN-01. The sequence alignment shows that the Val143 and Thr222 equivalent residues are replaced by bulkier Leu or Ile residues in several of the Mitogen Activated Protein Kinase families (Table 5). To investigate the effect of these bulkier side chains on the hydroxyl pocket, we starting from the PDK1 crystal structure, replaced residues Val143 with Ile and Thr222 with Leu in standard side chain rotamers (in O [24]), which indeed resulted in van der Waals clashes with C7 of staurosporine (shortest distances: 2.8 Å for Leu222, 3.5 Å for Ile143), and may therefore explain the lack of susceptibility towards UCN-01 in the Mitogen Activated Protein Kinase families. CDK2 is inhibited by both staurosporine and UCN-01 similarly, however this kinase lacks a hydrogen bonding partner for the 7-hydroxyl and contains a bulky Phe (Phe80) at the Leu159 equivalent position. In a superposition of CDK2-staurosporine structure [31] with PDK1-UCN-01 (RMSD = 1.3Å on Cα atoms) staurosporine is seen to be shifted by 1.2 Å out of the potential hydroxyl pocket due to presence of the bulky Phe80. Interaction of the 7-hydroxyl on UCN-01 was described to be water mediated in CDK2 due to the lack of hydrogen bonding residues [35]. This particular example highlights the limitations of the approach described above. Other examples where none of the described effects account for the observed behaviour are AMPK and

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MSK1. Both MSK1 and SGK1 show the same sequence in their hydroxyl-pocket with Thr406/Thr407, respectively, as potential hydrogen bonding partners, but both were placed in different groups. MSK1 activity is abolished by 1 μ M staurosporine, but shows residual activity (11 %) with UCN-01. SGK1 activity is at 25% of control activity with 1 μ M UCN-01, but twice as high with staurosporine.

Conclusions

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UCN-01 was subjected to a specificity analysis against an in-house panel of 29 protein kinases. Contrary to the suggestions of some previous reports. the data show that UCN-01 is not a specific inhibitor as it inhibited more than half of the tested kinases at significant levels. A direct comparison with staurosporine, however, showed a different pattern of inhibition, and was the subject of further analysis. We have reported the crystal structures of PDK1 in complex with the inhibitors staurosporine and UCN-01. Both inhibitors appear to bind to PDK1 in a similar fashion compared to the Chk1-UCN-01 or PKA-staurosporine [29] complex, with additional hydrogen bonding interactions at the UCN-01 7-hydroxyl group. This moiety is hydrogen bonded directly to Thr222 and indirectly via an ordered water molecule to Gln220. A different water-mediated hydrogen bonding network is also observed in other UCN-01 complexes known to date [35, 30], and might serve as a starting point for further structure-based optimisation. The residues around the 7-hydroxyl group ("hydroxylpocket") were aligned with known kinase structures and kinases sequences. It is apparent that spatial effects in the identified pocket play a key role in determining UCN-01 inhibition, as does the presence of hydrogen bonding partners for the additional hydroxyl group.

Table 3
Details of data collection & structure refinement. Values between brackets are for the highest resolution shell. Crystals were cryo-cooled to 100 K. All measured data were included in structure refinement.

Dataset	Staurosporine	UCN-01
Space group	P3 ₂ 21	P3 ₂ 21
Cell dimensions (Å)	a=124.17	a=123.39
	b=124.17	b=123.39
	c=47.31	c=47.12
Resolution range (Å)	25-2.30 (2.38-2.30)	25-2.50 (2.59-2.50)
# Observed reflections	31730 (3091)	68515 (6290)
# Unique reflections	18018 (1794)	14395 (1430)
Redundancy	1.8 (1.7)	4.8 (4.4)
Ι/σΙ	7.5 (1.8)	4.5 (2.6)
Completeness (%)	95.8 (95.8)	100.0 (99.9)
R _{merge}	0.096 (0.505)	0.167 (0.688)
R _{cryst} , R _{free}	0.218, 0.255	0.189, 0.257
RMSD from ideal		
geometry		
Bonds (Å)	0.007	0.009
Angles (°)	1.7	1.8
B-factor RMSD (Å)	1.5	1.4
(bonded, main chain)		
 protein (Å)	31.5	27.3
 inhibitor (Å)	18.5	17.4

Table 4

Hydrogen bonding between inhibitors and PDK1. Hydrogen bonds between PDK1 and UCN-01 / staurosporine (STO) were calculated with WHAT IF [36] using the HB2 algorithm [37]. This algorithm gives a 0 (no hydrogen bond) to 1 (optimal hydrogen bond) score to reflect hydrogen bond geometry (HB2 column), Donor-acceptor distances are also listed (D-A).

Inhibitor	Protein/H	UCN-01	UCN-01	STO D-A	STO	Comment
	₂ O	D-A (Å)	HB2	(Å)	HB2	
O5	N-	2.8	0.76	3.0	0.81	Conserved
	Ala162					
N6	O-Ser162	2.9	0.80	3.1	0.67	Conserved
N4'	0-	3.2	0.68	3.1	0.39	Conserved
	Glu209					
N4'	Οε2-	2.6	0.63	2.5	0.45	Conserved
	Glu166					
O7	Ογ1-	3.0	0.56			7-hydroxyl
	Thr222					
O7	H ₂ O	3.0	0.89			Water
						mediated to
						(Οε1-
						Gln220)

Table 5

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Comparison of inhibition by UCN-01 vs. staurosporine and hydroxyl pocket-lining residues.

The indicated protein kinases were assayed at 0.1 mM ATP as described previously [17, 26], in the absence or presence of 1μ M staurosporine (STO) or UCN-01. Results are presented as percentage of kinase activity compared to that in control incubations. The activity results displayed in the two columns are an average of a triplicate determination. Abbreviations not

defined in main text: ROCKII, Rho-dependent protein kinase-II; AMPK, AMP-activated protein kinase; MKK1, MAP-kinase kinase-I; PRAK, p38-regulated/activated protein kinase; PHK, phosphorylase kinase; CK2, Casein kinase-2; CHK1, cell cycle checkpoint kinase-1; DYRK, dual specificity tyrosine phosphorylated and regulated kinase; CSK, C-terminal Src kinase. Residues lining the hydroxyl pocket are shown in the last five columns, as derived from a multiple sequence alignment with T-Coffee [38].

Kinase STO $\frac{\text{UCN-}}{01}$

Both STO and UCN-01

inhibit

PDK1	5 . 1	0 + 1	Met13	Val14	Leu15	Gln22	Thr22
PDKI	5 ± 1	U±I	4	3	9	0	2
CHK1 (1NVQ [<u>30]</u>)	3 ± 1	1 ± 0	Ile	Val	Leu	Lys14 5	Ser147
ΡΚCα	8 ± 2	1 ± 0	Leu	Thr	Met	Lys	Ala
AMPK	0 ± 0	1 ± 1	Leu	Ile	Met	Lys	Ala
PHOS.KINASE (1PHK [39])	2 ± 3	1 ± 2	Leu	Ile	Phe	Lys	Thr
Lck (1QPJ [40])	0 ± 0	3 ± 1	Met	Val	Thr	Lys	Ala
CDK2/cyclin A (1AQ1 [31])	12 ± 12	8 ± 0	Leu	Val	Phe80	Lys	Ala
PKBΔPH (106K [<u>41</u>])	8 ± 2	9 ± 1	Leu	Thr	Met	Lys	Thr
ROCK-II	9 ± 5	13 ± 2	Met	Val	Met	Lys	Ala
S6K1	24 ± 8	21 ± 4	Leu	Val	Leu	Lys	Thr
GSK3β (1109 [<u>42</u>])	29 ± 6	25 ± 5	Met	Val	Leu	Lys	Cys
STO inhibits stronger than	1						
UCN-01							
MSK1	1 ± 0	11 ± 0	Leu	Val	Leu	Val	Thr40

					6
DYRK1α	2 ± 2 15 ± 2 Leu	Met	Phe	Lys	Val
PKA (1STC [29])	4 ± 1 27 ± 2 Leu	Val	Met13	Gln	Thr18
1111(1010 (22))	121 2122 200		4	0	3
MKK1	5 ± 8 53 ± 1 Leu	Val	Met	Lys	Cys
MAPKAP-K2	$23 \pm 1~60 \pm 1~His$	Val	Met	Lys	Thr
CSK (1BYG [43])	25 ± 8 58 ± 3 Met	Val	Thr	Lys	Ser
SAPK3/p38γ (1CM8 [<u>44</u>])	$37\pm0~94\pm8~Leu$	Ile	Met	Lys	Leu
SAPK4/p38δ	$40\pm5\ 100\pm7Leu$	Ile	Met	Lys	Leu
PRAK	48 ± 1 89 ± 4 His	Val	Met	Lys	Cys
UCN-01 inhibits stronge	r				
than STO					
MAPKAP-K1a	18 ± 1 ± 1 Leu	Val	Leu	T	Thr34
MAPKAP-K1a	10 1±1 Leu	vai	Leu	Lys	1
SGK1	51 ± 4 22 ± 4 Leu	Val	Leu	Val	Thr40
SOKI	31 1 4 22 1 4 Leu	v ai	Leu	v ai	7
Neither UCN-01 nor STC)				
inhibits					
MAPK2/ERK2 (1ERK [45])	100 ± 107 ± 5 Leu	Ile	Gln	Lys	Cys
Milit REFERRE (TERRE [<u>45]</u>)	4	110	Oiii	Lys	Cys
JNKSAPK1c	$91 \pm 3\ 112 \pm 6 \text{Met}$	Ile	Met	Lys	Leu
SAPK2α/p38 (1P38 [<u>46]</u>)	$76 \pm 4\ 107 \pm 5 \text{Leu}$	Ile	Thr	Lys	Leu
SAPK2β/p38β2	84 ± 106 ± 4 Leu	Ile	Thr	Arg	Leu
5AF K2p/p36p2	11	ne	1111	Aig	Leu
CK2 (1F0Q [47])	95 ± 4 Leu	Val	Phe	Arg	Ile
CK2 (110Q [<u>41]</u>)	11 Lea	v dl	1 116	Aug	ne
CK1 (1CKI [48])	95 ± 96 ± 0 Tyr	Pro	Met	Tyr	Ile
Citi (ICiti [<u>10]</u>)	11	110	iviet	1 y 1	110

NEK6 $\frac{109 \pm}{2} 80 \pm 7 \text{ Leu} \quad \text{Ile} \quad \text{Leu} \quad \text{Lys} \quad \text{Gly}$

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Example 7: Co-ordinates for PDK1 fragment co-crystallised with

Staurosporine

```
REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.30 A
   REMARK starting r= 0.2196 free r= 0.2545
    REMARK final
                   r= 0.2182 free r= 0.2553
    REMARK B rmsd for bonded mainchain atoms= 1.536 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.154 target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.576 target= 2.0
   REMARK B rmsd for angle sidechain atoms= 3.220 target= 2.5
    REMARK rweight= 0.1000 (with wa= 2.58634)
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 124.172 b= 124.172 c= 47.314 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1 : /ddl/david/projects/MY CNS/prot.par
    REMARK parameter file 2 : /ddl/david/projects/MY_CNS/sto.par
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : /ddl/david/projects/MY_CNS/glycerol.par
   REMARK molecular structure file: ../generate/alternate.mtf
    REMARK input coordinates: ../minimize/minimize.pdb
    REMARK reflection file= ../../1/hkl/cns.hkl
    REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.30
25
   REMARK initial B-factor correction applied to fobs :
    REMARK B11= -4.525 B22= -4.525 B33= 9.049
REMARK B12= -1.949 B13= 0.000 B23= 0.000
    REMARK B-factor correction applied to coordinate array B:
                                                                 -0.209
    REMARK bulk solvent: density level= 0.340909 e/A^3, B-factor= 36.8807
30
   A^2
    REMARK reflections with |Fobs|/sigma F < 0.0 rejected
    REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range:
                                                                    18858 (
    100.0 % )
   REMARK number of unobserved reflections (no entry or |F|=0):
                                                                       846 (
    4.5 %)
    REMARK number of reflections rejected:
                                                                         0 (
    0.0 %)
    REMARK total number of reflections used:
                                                                     18012 (
   95.5 % )
    REMARK number of reflections in working set:
                                                                     17259 (
    91.5 % )
    REMARK number of reflections in test set:
                                                                       753 (
    4.0 %)
   CRYST1 124.172 124.172 47.314 90.00 90.00 120.00 P 32 2 1
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE:30-Jan-2003 19:44:02
                                             created by user: david
    REMARK VERSION: 1.0
    ATOM
              1 CB PRO A 72
                                     64.267 -7.345 13.422 1.00 74.69 A
   ATOM
              2 CG PRO A 72
                                     63,278 -8,432 13,027 1,00 74,97 A
    ATOM
              3 C PRO A 72
                                    65.866 -6.007 12.013 1.00 73.72 A
    ATOM
              4 O PRO A 72
                                    66.500 -6.002 10.955 1.00 73.74 A
    ATOM
              5 N PRO A 72
                                    64.256 -7.651 11.034 1.00 74.67 A
    MOTA
              6 CD PRO A 72
                                    63.762 -8.901 11.640 1.00 75.33 A
55
             7 CA PRO A 72
                                    64.474 -6.639 12.090 1.00 74.30 A
    MOTA
             8 N GLNA 73
                                    66.329 -5.474 13.141 1.00 72.17 A
    ATOM
    ATOM
             9 CA GLN A 73
                                    67.635 -4.829 13.221 1.00 70.49 A
```

	MOTA	10	CB	GLN		73	67.570	-3.424	12.611	1.00 69.71 A
	MOTA	11	CG	GLN		73	66.670	-2.458	13.363	1.00 68.72 A
	MOTA	12	CD	GLN	Α	73	66.722	-1.054	12.795	0.00 69.01 A
	ATOM	13	OE1	GLN	A	73	67.785	-0.435	12.735	0.00 68.92 A
5	ATOM	14	NE2	GLN	Α	73	65.571	-0.541	12.376	0.00 68.92 A
	ATOM	15	C	GLN	A	73	68.057	-4.728	14.683	1.00 69.53 A
	ATOM	16	0	GLN	А	73	67.267	-5.015	15.585	1.00 69.69 A
	ATOM	17	N	PRO	А	74	69.313	-4.321	14.940	1.00 68.34 A
	ATOM	18	CD	PRO		74	70.411	-4.026	13.999	1.00 67.68 A
10	ATOM	19	CA	PRO		74	69.769	-4.204	16.330	1.00 67.15 A
	ATOM	20	СВ	PRO		74	71.198	-3.675	16.178	1.00 67.56 A
	ATOM	21	CG	PRO		74	71.635	-4.254	14.855	1.00 67.46 A
	ATOM	22	c	PRO		74	68.866	-3.240	17.105	1.00 65.27 A
	ATOM	23	ō	PRO		74	68.496	-2.186	16.584	1.00 65.27 A
15	ATOM	24	N	ARG		75	68.506	-3.598	18.337	1.00 63.27 A
13	ATOM	25	CA	ARG		75	67.642	-2.730	19.136	1.00 59.53 A
	ATOM	26	CB	ARG		75	67.543	-3.228	20.582	1.00 62.40 A
	ATOM	27	CG	ARG		75	66.120	-3.565	21.023	1.00 64.22 A
	ATOM	28	CD	ARG		75	66.020	-3.746	22.537	1.00 66.65 A
20	ATOM	29	NE	ARG		75	64.741	-4.332	22.943	1.00 68.76 A
	ATOM	30	CZ	ARG		75	64.390	-4.572	24.204	1.00 70.18 A
	MOTA	31		ARG		75	65.218	-4.272	25.197	1.00 70.31 A
	ATOM	32		ARG		75	63.213	-5.125	24.477	1.00 71.64 A
	MOTA	33	C	ARG	A	75	68.184	-1.306	19.126	1.00 55.61 A
25	ATOM	34	0	ARG	A	75	69.386	-1.082	18.961	1.00 55.58 A
	ATOM	35	N	LYS	A	76	67.294	-0.341	19.295	1.00 50.06 A
	ATOM	36	CA	LYS	A	76	67.704	1.050	19.297	1.00 45.50 A
	ATOM	37	CB	LYS	A	76	66.498	1.941	19.594	1.00 45.42 A
	ATOM	38	CG	LYS	A	76	66.404	3.192	18.735	1.00 45.70 A
30	ATOM	39	CD	LYS	A	76	66.329	2.829	17.257	1.00 44.53 A
	ATOM	40	CE	LYS	A	76	66.030	4.045	16.396	1.00 44.45 A
	ATOM	41	NZ	LYS	А	76	66.091	3.733	14.939	1.00 43.30 A
	ATOM	42	С	LYS	А	76	68.783	1.251	20.359	1.00 42.73 A
	ATOM	43	ō	LYS		76	68.715	0.681	21.447	1.00 42.46 A
35	ATOM	44	N	LYS		77	69.793	2.046	20.038	1.00 39.63 A
	ATOM	45	CA	LYS		77	70.851	2.309	20.995	1.00 36.33 A
	ATOM	46	CB	LYS		77	72.139	2.670	20.267	1.00 36.33 A
	ATOM	47	CG	LYS		77	72.655	1.570	19.353	1.00 36.55 A
	ATOM	48	CD	LYS		77	74.005	1.945	18.785	1.00 35.61 A
40	ATOM	49	CE	LYS		77	74.491	0.932	17.766	1.00 38.34 A
40	ATOM	50	NZ	LYS		77	74.706	-0.419	18.354	1.00 38.65 A
	ATOM	51	C	LYS		77	70.413	3.459	21.889	1.00 35.52 A
			0			77				
	ATOM	52		LYS			69.475	4.190	21.557	
4.5	ATOM	53	N	ARG		78	71.097	3.608	23.020	1.00 34.95 A
45	ATOM	54	CA	ARG		78	70.801	4.654	23.991	1.00 33.79 A
	ATOM	55	CB	ARG		78	69.917	4.094	25.114	1.00 35.78 A
	ATOM	56	CG	ARG		78	70.211	2.652	25.483	1.00 38.18 A
	ATOM	57	CD	ARG		78	69.036	2.040	26.239	1.00 38.81 A
	MOTA	58	NE	ARG		78	68.995	0.578	26.160	0.00 38.43 A
50	MOTA	59	CZ	ARG	Α	78	69.889	-0.232	26.719	0.00 38.44 A
	ATOM	60	NH1	ARG	Α	78	70.906	0.274	27.401	0.00 38.37 A
	ATOM	61	NH2	ARG	A	78	69.760	-1.549	26.610	0.00 38.37 A
	ATOM	62	C	ARG	Α	78	72.099	5.230	24.544	1.00 31.96 A
	ATOM	63	0	ARG	Α	78	73.133	4.576	24.515	1.00 32.75 A
55	ATOM	64	N	PRO	Α	79	72.060	6.470	25.055	1.00 30.51 A
	ATOM	65	CD	PRO		79	70.844	7.272	25.274	1.00 27.35 A
	ATOM	66	CA	PRO		79	73.236	7.150	25.611	1.00 29.82 A
	ATOM	67	CB	PRO		79	72.626	8.326	26.365	1.00 28.52 A
	ATOM	68	CG	PRO		79	71.418	8.628	25.559	1.00 29.89 A

		69	_		_	79		6.298	26.510	1.00 30.92 A
	ATOM	70	C	PRO		79	74.129 75.356	6.357		
	ATOM		0	PRO					26.412	
	MOTA	71	N	GLU		80	73.516	5.510	27.383	1.00 29.85 A
_	MOTA	72	CA	GLU		80	74.273	4.677	28.300	1.00 31.98 A
5	MOTA	73	CB	GLU		80	73.327	3.941	29.242	1.00 34.31 A
	MOTA	74	CG	GLU		80	72.697	2.710	28.622	1.00 41.92 A
	ATOM	75	CD	GLU		80	71.205	2.626	28.872	1.00 44.52 A
	MOTA	76		GLU		80	70.461	3.466	28.317	1.00 46.38 A
	MOTA	77	OE2	GLU		80	70.780	1.721	29.625	1.00 46.03 A
10	MOTA	78	C	GLU	Α	80	75.157	3.663	27.578	1.00 30.62 A
	MOTA	79	0	GLU	A	80	76.101	3.144	28.170	1.00 30.21 A
	MOTA	80	N	ASP	A	81	74.859	3.378	26.312	1.00 28.14 A
	MOTA	81	CA	ASP	A	81	75.659	2.417	25.548	1.00 27.32 A
	ATOM	82	CB	ASP	Α	81	74.938	1.990	24.253	1.00 27.75 A
15	ATOM	83	CG	ASP	A	81	73.612	1.275	24.512	1.00 30.45 A
	ATOM	84	OD1	ASP	A	81	73.495	0.549	25.525	1.00 30.76 A
	ATOM	85	OD2	ASP	A	81	72.686	1.424	23.686	1.00 30.74 A
	ATOM	86	С	ASP	A	81	77.026	2.990	25.166	1.00 26.35 A
	ATOM	87	0	ASP	A	81	77.895	2.266	24.680	1.00 25.33 A
20	ATOM	88	N	PHE	A	82	77.217	4.283	25.404	1.00 24.95 A
	ATOM	89	CA	PHE	А	82	78.457	4.948	25.035	1.00 23.57 A
	ATOM	90	CB	PHE		82	78,168	6.040	23.991	1.00 23.02 A
	ATOM	91	CG	PHE		82	77.507	5.534	22.742	1.00 23.64 A
	ATOM	92		PHE		82	78.270	5.059	21.680	1.00 23.15 A
25	ATOM	93	CD2	PHE		82	76.123	5.504	22.640	1.00 23.41 A
	ATOM	94	CE1	PHE		82	77.670	4.559	20.540	1.00 23.43 A
	ATOM	95	CE2	PHE		82	75.504	5.003	21.498	1.00 24.29 A
	ATOM	96	CZ	PHE		82	76.283	4.527	20.444	1.00 25.15 A
	ATOM	97	C	PHE		82	79.199	5.609	26.186	1.00 24.39 A
30	ATOM	98	ō	PHE		82	78.647	5.847	27.259	1.00 22.78 A
50	ATOM	99	N	LYS		83	80.471	5.896	25.932	1.00 22.40 A
	ATOM	100	CA	LYS		83	81.294	6.615	26.869	1.00 23.38 A
	ATOM	101	CB	LYS		83	82.554	5.834	27.250	1.00 24.29 A
	ATOM	101	CG	LYS		83	83.453	6.594	28.227	1.00 27.32 A
35	ATOM	102	CD	LYS		83	84.411	5.675	28.988	1.00 27.32 A
33	ATOM	103	CE	LYS		83	85.321	4.906	28.044	0.00 30.06 A
	ATOM	105	NZ	LYS		83	86.145	5.819	27.207	0.00 30.06 A
	ATOM	106	C	LYS	A	83 83	81.656 82.518	7.847	26.046	1.00 24.47 A 1.00 26.09 A
40	ATOM ATOM	107	N	LYS		84	80.965	8.951	25.162	1.00 26.09 A
40		108							25.583	
	ATOM	109	CA	PHE		84	81.211	10.182		
	ATOM	110	CB		A	84	80.073	11.169	25.811	1.00 20.62 A
	ATOM	111	CG	PHE		84	78.794	10.757	25.159	1.00 20.05 A
45	ATOM	112	CD1		A	84	77.915	9.905	25.805	1.00 18.27 A
45	ATOM	113	CD2	PHE		84	78.498	11.176	23.868	1.00 19.96 A
	MOTA	114	CE1		A	84	76.764	9.473	25.183	1.00 19.47 A
	MOTA	115	CE2	PHE		84	77.346	10.748	23.233	1.00 21.09 A
	MOTA	116	CZ	PHE		84	76.475	9.894	23.890	1.00 20.64 A
	MOTA	117	C	PHE		84	82.525	10.820	25.966	1.00 22.27 A
50	MOTA	118	0		A	84	82.900	10.822	27.129	1.00 24.09 A
	MOTA	119	N	GLY		85	83.213	11.371	24.972	1.00 22.72 A
	ATOM	120	CA	GLY		85	84.496	12.007	25.203	1.00 22.66 A
	ATOM	121	С	GLY		85	84.540	13.481	24.839	1.00 22.72 A
	MOTA	122	0	GLY	A	85	83.622	14.228	25.158	1.00 22.51 A
55	MOTA	123	N		А	86	85.608	13.894	24.162	1.00 22.49 A
	MOTA	124	CA	LYS		86	85.794	15.291	23.784	1.00 22.53 A
	MOTA	125	CB		Α	86	87.238	15.530	23.333	1.00 24.44 A
	ATOM	126	CG		A	86	87.617	14.804	22.051	1.00 26.94 A
	ATOM	127	CD	LYS	Α	86	89.033	15.120	21.594	1.00 29.52 A

	MOTA	128	CE	LYS	Α	86	89.166	16.571	21.154		35.93 A	
	MOTA	129	NZ	LYS	A	86	90.505	16.892	20.553	1.00	38.21 A	
	ATOM	130	C	LYS	Α	86	84.857	15.798	22.699	1.00	23.09 A	
	ATOM	131	0	LYS	A	86	84.295	15.032	21.923	1.00	22.85 A	
5	ATOM	132	N	ILE	А	87	84.702	17.114	22.664	1.00	22.28 A	
	MOTA	133	CA		A	87	83.867	17.780	21.683		21.22 A	
	ATOM	134	СВ		A	87	83.429	19.170	22.204		22.05 A	
	ATOM	135		ILE		87	82.792	19.993	21.076		17.65 A	
	ATOM	136		ILE		87	82.493	18.998	23.406		21.65 A	
10	ATOM	137		ILE		87	82.159	20.300	24.118		18.47 A	
	ATOM	138	C	ILE		87	84.707	17.963	20.418		21.83 A	
	ATOM	139	Ö	ILE		87	85.782	18.543	20.470		21.99 A	
	ATOM	140	N	LEU		88	84.226	17.463	19.288		22.57 A	
	ATOM	141	CA	LEU		88	84.964	17.614	18.039		22.76 A	
15	ATOM	142	CB	LEU		88	84.586	16.515	17.044		20.65 A	
13	ATOM	143	CG	LEU		88	84.899	15.107	17.535		20.03 A	
	ATOM	144		LEU		88	84.455	14.082	16.502		17.42 A	
				LEU			86.392		17.813			
	ATOM	145				88	84.657	15.004	17.428		17.76 A 23.53 A	
20	ATOM	146 147	C	LEU		88	85.512	18.964			24.73 A	
20	ATOM		0	LEU		88		19.577	16.794			
	MOTA	148	N	GLY		89	83.430	19.428	17.619		24.20 A	
	ATOM	149	CA	GLY		89	83.057	20.710	17.062		28.57 A	
	MOTA	150	С	GLY		89	81.649	21.131	17.431		32.57 A	
2.5	MOTA	151	0	GLY		89	80.834	20.318	17.882		32.78 A	
25	MOTA	152	N	GLU		90	81.363	22.412	17.224		35.17 A	
	MOTA	153	CA	GLU		90	80.063	22.964	17.542		39.17 A	
	MOTA	154	CB	GLU		90	80.168	23.853	18.784		41.47 A	
	MOTA	155	CG	GLU		90	80.112	23.061	20.082		47.18 A	
	MOTA	156	CD	GLU		90	80.422	23.893	21.313		50.49 A	
30	MOTA	157	OE1			90	81.610	24.228	21.526		51.41 A	
	MOTA	158	OE2			90	79.476	24.210	22.067		53.44 A	
	ATOM	159	C	GLU		90	79.436	23.743	16.402		40.69 A	
	MOTA	160	0	GLU		90	80.110	24.185	15.471		40.64 A	
	MOTA	161	N	GLY		91	78.121	23.881	16.488		42.58 A	
35	MOTA	162	CA	GLY		91	77.363	24.618	15.503		43.40 A	
	MOTA	163	C	GLY		91	76.303	25.335	16.306		44.83 A	
	ATOM	164	0	GLY	A	91	76.154	25.083	17.507	1.00	43.64 A	
	ATOM	165	N	SER	A	92	75.579	26.244	15.669	1.00	47.22 A	
	MOTA	166	CA	SER		92	74.522	26.969	16.366		48.94 A	
40	MOTA	167	CB	SER	A	92	73.961	28.066	15.461	1.00	51.50 A	
	MOTA	168	OG	SER	A	92	73.663	27.541	14.175	1.00	54.98 A	
	ATOM	169	C	SER		92	73.454	25.928	16.625		47.87 A	
	ATOM	170	0	SER	A	92	72.745	25.950	17.635	1.00	47.78 A	
	ATOM	171	N	PHE	A	93	73.392	24.994	15.689		46.49 A	
45	MOTA	172	CA	PHE	A	93	72.434	23.909	15.697		46.02 A	
	MOTA	173	CB	PHE	A	93	72.297	23.369	14.263	1.00	49.54 A	
	MOTA	174	CG	PHE	A	93	73.588	23.398	13.459	1.00	50.29 A	
	MOTA	175	CD1	PHE	A	93	74.301	22.229	13.209	1.00	52.29 A	
	MOTA	176	CD2	PHE	A	93	74.058	24.593	12.915	1.00	51.94 A	
50	MOTA	177	CE1	PHE	Α	93	75.459	22.245	12.424	1.00	52.28 A	
	ATOM	178	CE2	PHE	Α	93	75.209	24.622	12.135	1.00	52.58 A	
	ATOM	179	CZ	PHE	A	93	75.911	23.443	11.887	1.00	53.99 A	
	ATOM	180	C	PHE		93	72.700	22.754	16.662		43.48 A	
	ATOM	181	0	PHE		93	71.772	22.245	17.292		42.15 A	
55	ATOM	182	N	SER		94	73.955	22.343	16.796		39.99 A	
	ATOM	183	CA	SER		94	74.245	21.206	17.655		36.12 A	
	ATOM	184	СВ	SER		94	73.839	19.937	16.921		38.79 A	
	ATOM	185	OG	SER		94	74.549	19.863	15.695		40.39 A	
	ATOM	186	C	SER		94	75.697	21.066	18.083		32.29 A	

	ATOM	187	0	SER	Α	94	76.513	21.962	17.890	1.00	30.04 A
	ATOM	188	N	THR	Α	95	76.006	19.909	18.655	1.00	28.50 A
	ATOM	189	CA	THR	Α	95	77.350	19.614	19.116	1.00	26.86 A
	ATOM	190	CB	THR	Α	95	77.432	19.642	20.652	1.00	27.90 A
5	ATOM	191	OG1	THR	Α	95	76.907	20.882	21.136	1.00	32.56 A
	ATOM	192	CG2	THR	Α	95	78.874	19.502	21.112	1.00	27.77 A
	ATOM	193	C	THR		9.5	77.757	18.225	18.653		23.70 A
	ATOM	194	0	THR	А	95	76.971	17.287	18.724	1.00	24.35 A
	ATOM	195	N	VAL		96	78.991	18.100	18.184		22.75 A
10	ATOM	196	CA	VAL		96	79.505	16.813	17.733		20.60 A
	ATOM	197	CB	VAL		96	80.139	16.909	16.336		17.79 A
	ATOM	198		VAL		96	80.625	15.530	15.898		18.21 A
	ATOM	199	CG2	VAL		96	79.131	17.447	15.344		13.79 A
	ATOM	200	C	VAL		96	80.566	16.351	18.716		21.23 A
15	ATOM	201	ō	VAL		96	81.600	17.006	18.889		22.12 A
	ATOM	202	N	VAL		97	80.310	15.220	19.362		22.06 A
	ATOM	203	CA	VAL		97	81.244	14.690	20.345		24.07 A
	ATOM	204	CB	VAL		97	80.592	14.680	21.743		24.91 A
	ATOM	205		VAL		97	79.199	14.124	21.649		28.97 A
20		205	CG2			97	81.422	13.859	22.715		27.97 A
20	ATOM	205		VAL		97	81.748	13.859	20.002		
	ATOM		C								
	ATOM	208	0	VAL		97	81.017	12.491	19.436		26.62 A
	ATOM	209	N	LEU		98	83.007	13.024	20.329		22.92 A
	MOTA	210	CA	LEU		98	83.586	11.713	20.063		23.27 A
25	MOTA	211	CB	LEU		98	85.117	11.777	20.110		21.94 A
	MOTA	212	CG	LEU		98	85.932	10.495	19.854		22.83 A
	MOTA	213		LEU		98	85.606	9.924	18.486		23.24 A
	MOTA	214		LEU		98	87.422	10.802	19.945		21.21 A
	MOTA	215	С	LEU		98	83.069	10.782	21.144		23.95 A
30	MOTA	216	0	LEU		98	83.143	11.099	22.322		26.02 A
	MOTA	217	N	ALA		99	82.523	9.645	20.738		24.41 A
	ATOM	218	CA	ALA		99	81.999	8.677	21.686		23.76 A
	MOTA	219	CB	ALA		99	80.485	8.692	21.668		20.64 A
	MOTA	220	C	ALA		99	82.502	7.282	21.357		26.42 A
35	ATOM	221	0	ALA		99	82.792	6.951	20.195		26.78 A
	ATOM	222	N	ARG			82.602	6.462	22.394		26.77 A
	MOTA	223	CA	ARG	Α	100	83.055	5.094	22.238	1.00	26.80 A
	MOTA	224	CB	ARG			84.362	4.897	23.001		28.29 A
	MOTA	225	CG	ARG	A	100	84.967	3.522	22.853	1.00	33.87 A
40	MOTA	226	CD	ARG	Α	100	86.281	3.447	23.617	1.00	38.01 A
	MOTA	227	NE	ARG	Α	100	87.337	4.240	22.983	1.00	41.22 A
	MOTA	228	CZ	ARG	Α	100	87.932	3.917	21.837	1.00	41.46 A
	ATOM	229	NH1	ARG	Α	100	87.580	2.813	21.190	1.00	41.28 A
	MOTA	230	NH2	ARG	Α	100	88.887	4.692	21.339	1.00	43.39 A
45	ATOM	231	С	ARG	Α	100	81.970	4.167	22.770	1.00	24.32 A
	ATOM	232	0	ARG	Α	100	81.583	4.251	23.934	1.00	25.42 A
	ATOM	233	N	GLU	Α	101	81.456	3.308	21,900	1.00	22.41 A
	ATOM	234	CA	GLU	Α	101	80.417	2.367	22.281	1.00	22.87 A
	MOTA	235	CB	GLU	А	101	79.787	1.775	21.025	1.00	21.96 A
50	MOTA	236	CG	GLU			78.819	0.652	21.292		24.68 A
	ATOM	237	CD	GLU			78.203	0.137	20.018		28.27 A
	ATOM	238		GLU			78.965	-0.113	19.057		28.96 A
	ATOM	239	OE2	GLU			76.963	-0.022	19.971		29.77 A
	ATOM	240	C	GLU		101	81.015	1.261	23.151	1.00	
55	ATOM	241	o	GLU			81.945	0.574	22.738	1.00	
	ATOM	242	N	LEU			80.475	1.088	24.351		26.09 A
	ATOM	243	CA	LEU		102	80.982	0.083	25.289		28.74 A
	ALON	243	OM	טמע	1.7	102	00.902	0.003	25.205	1.00	20.79 A
	ATOM	244	СВ	LEU	a	102	80.173	0.110	26.593	1 00	30.16 A
	ALOM	744	CD	шы	r	102	00.1/3	0.110	20.353	1.00	30.10 A

	MOTA	245	CG	LEU A			80.347	1.308	27.532	1.00 34.19 A
	MOTA	246		LEU A			81.824	1.692	27.599	1.00 33.27 A
	ATOM	247	CD2	LEU A			79.527	2.477	27.046	1.00 34.46 A
	MOTA	248	C	LEU A			81.042	-1.359	24.791	1.00 28.32 A
5	ATOM	249	0	LEU Z	. 10)2	82.067	-2.024	24.916	1.00 29.83 A
	MOTA	250	N	ALA A	10)3	79.948	-1.841	24.226	1.00 27.34 A
	ATOM	251	CA	ALA A	. 10	0.3	79.887	-3.218	23.763	1.00 27.81 A
	ATOM	252	CB	ALA A			78.466	-3.549	23.367	1.00 27.48 A
	ATOM	253	С	ALA A			80.828	-3.593	22.624	1.00 27.42 A
10	ATOM	254	ō	ALA A			81.172	-4.765	22.463	1.00 28.68 A
	ATOM	255	N	THR A			81.257	-2.612	21.842	1.00 24.97 A
	ATOM	256	CA	THR A			82.105	-2.907	20.695	1.00 23.79 A
	ATOM	257	CB	THR A			81.441	-2.472	19.393	1.00 22.01 A
	ATOM	258		THR A			81.355	-1.041	19.379	1.00 23.91 A
15	ATOM	259	CG2				80.051	-3.069	19.261	1.00 23.31 A
13	ATOM	260	C	THR A			83.444	-2.221	20.712	1.00 17.30 A
	MOTA	261	0	THR A			84.350	-2.616	19.972	1.00 25.02 A
	MOTA	262	N	SER A			83.551	-1.172	21.525	1.00 24.89 A
20	MOTA	263	CA	SER A			84.775	-0.394	21.616	1.00 24.55 A
20	MOTA	264	CB	SER A			85.979	-1.334	21.732	1.00 26.36 A
	MOTA	265	OG	SER A			87.143	-0.621	22.090	1.00 32.45 A
	MOTA	266	C	SER A			84.916	0.514	20.374	1.00 23.38 A
	MOTA	267	0	SER A			85.931	1.175	20.188	1.00 24.92 A
	MOTA	268	N	ARG A			83.888	0.546	19.531	1.00 20.51 A
25	ATOM	269	CA	ARG A			83.906	1.372	18.323	1.00 19.31 A
	MOTA	270	CB	ARG A			82.778	0.947	17.370	1.00 19.05 A
	ATOM	271	CG	ARG A			83.099	-0.283	16.520	1.00 15.69 A
	MOTA	272	CD	ARG A	10	06	81.853	-0.804	15.832	1.00 19.45 A
	ATOM	273	NE	ARG A	. 10)6	82.144	-1.838	14.846	1.00 20.98 A
30	ATOM	274	CZ	ARG A	. 10)6	81.234	-2.673	14.354	1.00 21.77 A
	ATOM	275	NH1	ARG A	10)6	79.974	-2.599	14.768	1.00 19.65 A
	ATOM	276	NH2	ARG A	10)6	81.577	-3.560	13.427	1.00 21.43 A
	ATOM	277	C	ARG A	10)6	83.760	2.858	18.624	1.00 17.84 A
	ATOM	278	0	ARG A	10	06	83.022	3.234	19.525	1.00 15.87 A
35	ATOM	279	N	GLU A			84.463	3.691	17.863	1.00 18.23 A
	ATOM	280	CA	GLU Z			84.395	5.144	18.039	1.00 22.75 A
	ATOM	281	СВ	GLU Z			85.773	5.800	17.929	1.00 23.58 A
	ATOM	282	CG	GLU Z			86.828	5.254	18.859	1.00 32.15 A
	ATOM	283	CD	GLU A			88.066	6.131	18.878	1.00 35.04 A
40	ATOM	284		GLU A			88.145	7.019	19.755	1.00 36.99 A
	ATOM	285		GLU Z			88.949	5.944	18.007	1.00 37.54 A
	ATOM	286	C	GLU A			83.514	5.787	16.982	1.00 21.00 A
	ATOM	287	Ö	GLU A			83.709	5.577	15.787	1.00 21.37 A
	ATOM	288	N	TYR A			82.570	6.593	17.437	1.00 21.37 A
45	ATOM	289	CA	TYR A			81.652	7.298	16.559	1.00 19.40 A
43			CB	TYR A			80.228	6.791	16.754	1.00 18.30 A
	MOTA	290		TYR A						1.00 17.52 A 1.00 22.75 A
	MOTA	291	CG				79.993	5.373	16.309	
	MOTA	292		TYR A			79.727	5.075	14.972	1.00 20.94 A
	MOTA	293		TYR A			79.492	3.765	14.571	1.00 23.91 A
50	MOTA	294		TYR A			80.019	4.324	17.231	1.00 19.41 A
	MOTA	295	CE2	TYR A			79.788	3.026	16.845	1.00 19.33 A
	MOTA	296	CZ	TYR A			79.527	2.744	15.521	1.00 23.13 A
	MOTA	297	OH	TYR A			79.333	1.438	15.143	1.00 23.65 A
	MOTA	298	C	TYR A			81.660	8.777	16.906	1.00 18.00 A
55	MOTA	299	0	TYR A			81.929	9.161	18.046	1.00 18.12 A
	MOTA	300	N	ALA A			81.370	9.603	15.912	1.00 17.20 A
	ATOM	301	CA	ALA A	10	9	81.274	11.036	16.114	1.00 15.30 A
	ATOM	302	CB	ALA A	10	9	81.853	11.784	14.928	1.00 13.44 A
	MOTA	303	C	ALA A	10	9	79.759	11.205	16.178	1.00 17.20 A

	MOTA	304	0	ALA A		79.0		11.019	15.179		17.23 A	
	MOTA	305	N	ILE A		79.2		11.522	17.362		17.40 A	
	MOTA	306	CA	ILE A		77.1		11.654	17.542		17.60 A	
	MOTA	307	CB	ILE A		77.		10.957	18.842		16.56 A	
	5 ATOM	308		ILE A		75.		11.236	19.119		14.97 A	
	MOTA	309	CG1	ILE A	110	77.		9.453	18.728	1.00	14.02 A	
	ATOM	310	CD1	ILE A	110	77.	197	8.632	19.907	1.00	11.93 A	
	MOTA	311	C	ILE A	110	77.	306	13.089	17.548	1.00	19.83 A	
	ATOM	312	0	ILE A	110	77.	690	13.892	18.396	1.00	20.84 A	
1	MOTA 0	313	N	LYS A	111	76.	444	13.415	16.597	1.00	18.58 A	
	ATOM	314	CA	LYS A	111	75.	902	14.761	16.551	1.00	20.88 A	
	ATOM	315	CB	LYS A	111	75.	455	15.115	15.131	1.00	21.39 A	
	ATOM	316	CG	LYS A	111	75.0	016	16.558	14.975	1.00	24.84 A	
	ATOM	317	CD	LYS A	111	75.0	005	16.971	13.516	1.00	27.43 A	
1	5 ATOM	318	CE	LYS A		74.	426	18.359	13.343	1.00	28.44 A	
	ATOM	319	NZ	LYS A	111	74.	619	18.871	11.972	1.00	28.27 A	
	ATOM	320	С	LYS A		74.		14.819	17.507		20.66 A	
	ATOM	321	ō	LYS A		73.		14.008	17.410		20.23 A	
	ATOM	322	N	ILE A		74.		15.765	18.441		20.09 A	
2	MOTA 0	323	CA	ILE A		73.		15.914	19.426		23.02 A	
	ATOM	324	CB	ILE A		74.3		15.882	20.863		24.20 A	
	ATOM	325		ILE A		73.		15.765	21.864		21.42 A	
	ATOM	326		ILE A		75.2		14.692	21.023		24.14 A	
	ATOM	327		ILE A		75.1		14.634	22.375		26.83 A	
2	5 ATOM	328	C	ILE A		72.		17.225	19.221		22.53 A	
-	ATOM	329	ŏ	ILE A		73.		18.286	19.132		21.31 A	
	ATOM	330	N	LEU A		71.		17.138	19.150		24.04 A	
	ATOM	331	CA	LEU A		70.1		18.313	18.940		25.81 A	
	ATOM	332	CB	LEU A		70.		18.264	17.555		24.66 A	
	MOTA 0		CG	LEU A		70.		18.095	16.295		26.73 A	
-	ATOM	334		LEU A		71.		16.620	16.093		24.51 A	
	ATOM	335		LEU A		70.		18.637	15.083		26.16 A	
	ATOM	336	C	LEU A		69.		18.400	19.994		27.62 A	
	ATOM	337	0	LEU A		69.1		17.398	20.314		29.70 A	
2	5 ATOM	338	N	GLU A		69.		19.597	20.530		29.70 A	
	ATOM	339	CA	GLU A		68.		19.806	21.526		31.56 A	
	ATOM	340	CB	GLU A		68.		21.020	22.391		34.85 A	
	ATOM	341	CG	GLU A		67.		21.357	23.392		42.32 A	
	ATOM	342	CD	GLU A		67.		22.670	24.108		45.56 A	
	MOTA 0	343		GLU A		68.0		23.700	23.417		48.01 A	
-	MOTA ON	344		GLU A		67.		22.673	25.359		48.10 A	
	ATOM	345	C	GLU A		67.		20.036	20.816		31.02 A	
	ATOM	346	o	GLU A		66.		21.049	20.310		30.39 A	
						66.			20.140			
	ATOM 5 ATOM	347 348	N CA	LYS A		64.1		19.099 19.218	20.321		30.58 A 31.63 A	
-		349	CB						20.321		28.91 A	
	ATOM		CG	LYS A		63.		18.049				
	ATOM	350 351	CD	LYS A		64.2		16.742 15.580	20.003		28.07 A	
	ATOM					63.			20.368		23.95 A	
	MOTA 03	352	CE	LYS A		63.7		14.960	21.707		23.89 A	
-			NZ	LYS A		62.1		13.782	22.020		24.15 A	
	ATOM	354	C	LYS A		64.		20.551	20.591		33.78 A	
	MOTA	355	0	LYS A		63.4		21.100	19.711		33.61 A	
	ATOM	356	N	ARG A		64.		21.076	21.801		35.55 A	
	ATOM	357	CA	ARG A		63.		22.332	22.176		38.66 A	
2	5 ATOM	358	CB	ARG A		63.		22.627	23.663		42.20 A	
	ATOM	359	CG	ARG A		62.		23.603	24.302		47.35 A	
	ATOM	360	CD	ARG A		63.		24.685	25.109		52.44 A	
	ATOM	361	NE	ARG A		64.		24.141	26.166		56.30 A	
	MOTA	362	CZ	ARG A	. 116	64.	142	23.920	27.423	1.00	57.97 A	

	ATOM	363	NH1	ARG	Α	116	62.899	24.199	27.808	1.00	58.89 A
	ATOM	364		ARG			65.006	23.420	28.300		56.55 A
	ATOM	365	C	ARG			64.227	23.472	21.323		37.67 A
	ATOM	366	ō	ARG			63.474	24.246	20.735		36.66 A
5	ATOM	367	N	HIS			65.550	23.555	21.259		37.78 A
,	ATOM	368	CA	HIS			66.236	24.590	20.501		35.88 A
	ATOM	369	CB	HIS			67.744	24.417	20.676		35.60 A
	MOTA	370	CG	HIS			68.560	25.532	20.101		37.06 A
	MOTA	371		HIS			69.508	25.535	19.134		38.11 A
10	MOTA	372		HIS			68.469	26.831	20.550		37.56 A
	ATOM	373		HIS			69.325	27.587	19.886		38.35 A
	ATOM	374	NE2	HIS	Α	117	69.969	26.825	19.021	1.00	38.67 A
	MOTA	375	C	HIS	Α	117	65.859	24.529	19.024	1.00	34.83 A
	ATOM	376	0	HIS	Α	117	65.600	25.554	18.398	1.00	35.80 A
15	ATOM	377	N	ILE	Α	118	65.827	23.321	18.474	1.00	33.01 A
	MOTA	378	CA	ILE	Α	118	65.483	23.122	17.071	1.00	32.12 A
	ATOM	379	CB	ILE			65.575	21.629	16.692	1.00	33.37 A
	ATOM	380	CG2	ILE			64.968	21.398	15.312		33.44 A
	ATOM	381		ILE			67.032	21.168	16.732		33.47 A
20	ATOM	382		ILE			67.195	19.685	16.479		35.01 A
20	ATOM	383	C	ILE			64.066	23.603	16.760		31.17 A
	ATOM	384	Ö	ILE		118	63.838	24.295	15.774		29.39 A
	ATOM	385	N	ILE			63.117	23.209	17.600		31.17 A
	MOTA	386	CA	ILE			61.725	23.590	17.420		31.73 A
25	MOTA	387	CB	ILE			60.841	22.896	18.473		31.45 A
	MOTA	388		ILE			59.471	23.560	18.548		26.98 A
	MOTA	389		ILE			60.735	21.409	18.131		27.55 A
	ATOM	390		ILE			60.092	20.574	19.205		26.52 A
	MOTA	391	C	ILE	Α	119	61.549	25.100	17.519	1.00	33.53 A
30	MOTA	392	0	ILE	Α	119	60.879	25.714	16.688	1.00	32.81 A
	ATOM	393	N	ALA	Α	120	62.165	25.691	18.535	1.00	34.30 A
	ATOM	394	CA	ALA	Α	120	62.078	27.125	18.749	1.00	34.63 A
	ATOM	395	CB	ALA	А	120	62.811	27.506	20.029	1.00	35.03 A
	ATOM	396	С	ALA			62.657	27.889	17.574	1.00	35.68 A
35	ATOM	397	ō	ALA			62.141	28.938	17.195		36.85 A
-	ATOM	398	N	GLU			63.732	27.369	16.995		35.66 A
	ATOM	399	CA	GLU			64.375	28.041	15.870		36.43 A
	ATOM	400	CB	GLU			65.873	27.726	15.864		40.99 A
	ATOM	401	CG	GLU			66.637	28.166	17.116		45.01 A
40									17.205		
40	ATOM	402	CD	GLU			66.844	29.676			48.12 A
	MOTA	403		GLU			67.670	30.104	18.043		49.33 A
	MOTA	404	OE2	GLU			66.188	30.433	16.451		49.20 A
	MOTA	405	C	GLU			63.780	27.670	14.512		34.98 A
	MOTA	406	0	GLU			64.282	28.105	13.480		34.50 A
45	MOTA	407	N	ASN			62.716	26.869	14.517		33.68 A
	ATOM	408	CA	ASN	Α	122	62.060	26.434	13.286	1.00	32.99 A
	MOTA	409	CB	ASN	Α	122	61.492	27.639	12.530	1.00	35.58 A
	ATOM	410	CG	ASN	Α	122	60.424	28.373	13.315	1.00	38.88 A
	ATOM	411	OD1	ASN	Α	122	60.717	29.154	14.227	1.00	38.30 A
50	ATOM	412		ASN			59.170	28.116	12.970	1.00	38.77 A
	ATOM	413	C	ASN			63.024	25.679	12.367		31.80 A
	ATOM	414	ŏ	ASN			63.095	25.957	11.172		30.78 A
	ATOM	415	N	LYS			63.754	24.716	12.919		29.93 A
	ATOM	416	CA	LYS			64.717	23.966	12.120		29.87 A
55	ATOM	417	CB	LYS			66.100	24.016	12.775		30.75 A
55	ATOM	418	CG	LYS			66.669	25.406	12.895		33.94 A
		418	CD						11.527		
	ATOM			LYS			66.810	26.049			
	MOTA	420	CE	LYS			67.354	27.466	11.646		39.07 A
	ATOM	421	NZ	LYS	Α	123	67.460	28.121	10.310	1.00	41.71 A

	ATOM	422	C	LYS	Α	123	64.337	22.514	11.880	1.00 27.38 A
	ATOM	423	0	LYS	Α	123	65.139	21.745	11.355	1.00 24.93 A
	ATOM	424	N	VAL	Α	124	63.124	22.132	12.260	1.00 24.22 A
	ATOM	425	CA	VAL			62.716	20.756	12.062	1.00 22.73 A
5	ATOM	426	CB	VAL			61.235	20.559	12.416	1.00 22.36 A
-	MOTA	427		VAL			60.794	19.146	12.064	1.00 22.84 A
	ATOM	428	CG2	VAL			61.031	20.802	13.905	1.00 20.63 A
	MOTA	429	C	VAL			62.981	20.320	10.623	1.00 23.50 A
	MOTA	430	0	VAL			63.633	19.297	10.385	1.00 21.86 A
10	ATOM	431	N	PRO			62.512	21.109	9.639	1.00 23.91 A
	MOTA	432	CD	PRO	Α	125	61.806	22.399	9.725	1.00 24.52 A
	ATOM	433	CA	PRO	Α	125	62.737	20.736	8.239	1.00 24.57 A
	MOTA	434	CB	PRO	Α	125	62.147	21.914	7.464	1.00 23.69 A
	ATOM	435	CG	PRO			61.098	22.450	8.400	1.00 25.18 A
15	ATOM	436	c	PRO			64.217	20.520	7.923	1.00 23.84 A
	ATOM	437	ō	PRO			64.568	19.618	7.172	1.00 22.92 A
		438	N	TYR			65.073	21.353	8.501	1.00 24.86 A
	MOTA									
	MOTA	439	CA	TYR			66.511	21.259	8.274	1.00 28.10 A
	MOTA	440	CB	TYR			67.202	22.494	8.859	1.00 32.76 A
20	ATOM	441	CG	TYR			66.802	23.766	8.146	1.00 39.46 A
	ATOM	442	CD1	TYR	Α	126	67.466	24.179	6.987	1.00 42.04 A
	MOTA	443	CE1	TYR	Α	126	67.063	25.322	6.292	1.00 43.67 A
	ATOM	444	CD2	TYR	Α	126	65.722	24.531	8.597	1.00 42.16 A
	ATOM	445	CE2	TYR	А	126	65.309	25.673	7.909	1.00 43.70 A
25	ATOM	446	CZ	TYR			65.983	26.062	6.758	1.00 44.51 A
	ATOM	447	OH	TYR			65.570	27.183	6.068	1.00 45.30 A
	ATOM	448	C	TYR			67.115	19.984	8.852	1.00 26.14 A
	ATOM	449	Ö	TYR			67.768	19.225	8.141	1.00 26.15 A
	ATOM	450		VAL			66.891	19.756	10.141	1.00 24.35 A
20			N							
30	MOTA	451	CA	VAL			67.396	18.568	10.819	1.00 24.93 A
	MOTA	452	CB	VAL			66.956	18.568	12.296	1.00 24.24 A
	ATOM	453		VAL			67.444	17.316	12.997	1.00 23.36 A
	ATOM	454		VAL			67.492	19.809	12.979	1.00 21.11 A
	MOTA	455	C	VAL	Α	127	66.894	17.290	10.130	1.00 25.81 A
35	ATOM	456	0	VAL	Α	127	67.655	16.351	9.903	1.00 25.79 A
	ATOM	457	N	THR	Α	128	65.612	17.273	9.793	1.00 25.57 A
	ATOM	458	CA	THR	А	128	64.996	16.136	9.114	1.00 26.36 A
	MOTA	459	CB	THR	А	128	63.486	16.384	8.908	1.00 25.21 A
	ATOM	460		THR			62.827	16.390	10.181	1.00 29.29 A
40	ATOM	461		THR			62.883	15.317	8.043	1.00 25.73 A
	ATOM	462	C	THR			65.640	15.898	7.748	1.00 26.97 A
	ATOM	463	o	THR			65.929	14.760	7.366	1.00 25.68 A
			N							
	MOTA	464		ARG			65.854	16.980	7.012	1.00 27.23 A
	MOTA	465	CA	ARG			66.462	16.897	5.692	1.00 29.37 A
45	MOTA	466	CB	ARG			66.484	18.282	5.032	1.00 32.35 A
	ATOM	467	CG	ARG			66.936	18.280	3.583	1.00 36.81 A
	MOTA	468	CD	ARG	Α	129	67.208	19.693	3.064	1.00 40.45 A
	MOTA	469	NE	ARG	Α	129	66.178	20.651	3.459	1.00 44.54 A
	MOTA	470	CZ	ARG	Α	129	64.874	20.474	3.268	1.00 48.21 A
50	ATOM	471	NH1	ARG	Α	129	64.431	19.366	2.681	1.00 50.01 A
	ATOM	472	NH2	ARG	А	129	64.008	21.403	3.668	1.00 47.79 A
	ATOM	473	C	ARG			67.884	16.379	5.828	1.00 28.98 A
	ATOM	474	ō	ARG			68.316	15.532	5.054	1.00 28.26 A
	ATOM	475	N	GLU			68.606	16.895	6.822	1.00 29.28 A
55	ATOM	476	CA	GLU			69.988	16.490	7.057	1.00 29.28 A
23										
	MOTA	477	CB	GLU			70.556	17.203	8.287	1.00 34.18 A
	MOTA	478	CG	GLU		130	72.078	17.220	8.344	1.00 38.81 A
	ATOM	479	CD	GLU			72.633	17.650	9.702	1.00 41.66 A
	ATOM	480	OE1	GLU	Α	130	71.946	18.408	10.427	1.00 42.36 A

	MOTA	481	OE2	GLU 2	A	130	73.771	17.236	10.035	1.00 42.31 A
	ATOM	482	C	GLU 2	A	130	70.063	14.984	7.273	1.00 30.12 A
	ATOM	483	0	GLU 2	A	130	70.861	14.298	6.638	1.00 29.62 A
	ATOM	484	N	ARG 2	A	131	69.228	14.474	8.173	1.00 29.21 A
5	ATOM	485	CA	ARG 2			69.215	13.046	8.458	1.00 30.93 A
	ATOM	486	CB	ARG A			68.241	12.724	9.601	1.00 32.88 A
	ATOM	487	CG	ARG A			68.035	11.223	9.795	1.00 36.48 A
	ATOM	488	CD	ARG I			67.069	10.885	10.922	1.00 41.14 A
	ATOM	489	NE	ARG 2			66.859	9.440	11.012	1.00 45.98 A
10	MOTA	490	CZ	ARG 2			66.167	8.833	11.974	1.00 48.77 A
	ATOM	491		ARG 2			65.605	9.546	12.946	1.00 48.39 A
	ATOM	492	NH2	ARG 2	A	131	66.045	7.509	11.968	1.00 48.16 A
	MOTA	493	C	ARG 2	Ą	131	68.836	12.226	7.224	1.00 29.97 A
	ATOM	494	0	ARG 2	A	131	69.398	11.157	6.986	1.00 28.24 A
15	ATOM	495	N	ASP 2	Ą	132	67.889	12.725	6.437	1.00 28.56 A
	ATOM	496	CA	ASP 2			67.460	11.996	5.251	1.00 29.18 A
	ATOM	497	CB	ASP 2			66.160	12.583	4.710	1.00 31.39 A
	ATOM	498	CG	ASP I			65.005	12.409	5.682	1.00 38.76 A
	ATOM	499		ASP I			64.892	11.319	6.283	1.00 38.76 A
20										
20	MOTA	500		ASP 2			64.206	13.355	5.846	1.00 44.19 A
	MOTA	501	C	ASP 2			68.510	11.936	4.150	1.00 27.67 A
	MOTA	502	0	ASP I			68.688	10.896	3.522	1.00 27.56 A
	ATOM	503	N	VAL 2			69.200	13.044	3.909	1.00 26.09 A
	MOTA	504	CA	VAL 2			70.232	13.063	2.886	1.00 25.09 A
25	MOTA	505	CB	VAL 2	A	133	70.859	14.459	2.742	1.00 25.26 A
	ATOM	506	CG1	VAL 2	A	133	72.157	14.369	1.961	1.00 24.32 A
	ATOM	507	CG2	VAL 2	A	133	69.890	15.390	2.029	1.00 24.76 A
	ATOM	508	C	VAL 2	A	133	71.320	12.076	3.266	1.00 25.33 A
	ATOM	509	0	VAL 2			71.742	11.270	2.445	1.00 23.59 A
30	ATOM	510	N	MET 2			71.764	12.138	4.520	1.00 26.01 A
	ATOM	511	CA	MET 2			72.812	11.243	4.995	1.00 27.63 A
	ATOM	512	CB	MET 2			73.210	11.576	6.436	1.00 25.11 A
	ATOM	513	CG	MET 2			74.056	12.834	6.539	1.00 23.11 A
	ATOM	514	SD	MET						1.00 27.32 A
2.5							74.875	13.035	8.132	
35	MOTA	515	CE	MET :			73.545	13.741	9.104	1.00 28.66 A
	ATOM	516	C	MET 2			72.431	9.779	4.901	1.00 28.59 A
	MOTA	517	0	MET 2			73.276	8.938	4.599	1.00 31.12 A
	ATOM	518	N	SER A			71.168	9.467	5.165	1.00 29.14 A
	MOTA	519	CA	SER 3	A	135	70.709	8.082	5.090	1.00 31.93 A
40	ATOM	520	CB	SER 2	A	135	69.261	7.966	5.558	1.00 32.44 A
	ATOM	521	OG	SER 2	A	135	69.112	8.470	6.868	1.00 40.09 A
	ATOM	522	C	SER 2	A	135	70.786	7.557	3.668	1.00 31.36 A
	ATOM	523	0	SER 2	A	135	71.010	6.374	3.454	1.00 32.23 A
	ATOM	524	N	ARG 2			70.597	8.448	2.701	1.00 31.66 A
45	ATOM	525	CA	ARG 2			70.602	8.075	1.293	1.00 32.53 A
	ATOM	526	CB	ARG 2			69.798	9.095	0.491	1.00 33.51 A
	ATOM	527	CG	ARG I			68.361	9.274	0.962	1.00 38.41 A
	ATOM	528	CD	ARG A			67.676	10.352	0.137	1.00 30.41 A
			NE							
50	ATOM	529		ARG I			67.850	10.090	-1.288	1.00 42.75 A
50	MOTA	530	CZ	ARG 2			67.560	10.953	-2.253	1.00 44.58 A
	MOTA	531		ARG 2			67.071	12.151	-1.950	1.00 45.74 A
	MOTA	532		ARG 2			67.771	10.621	-3.522	1.00 43.43 A
	MOTA	533	C	ARG 2			71.985	7.946	0.670	1.00 32.09 A
	MOTA	534	0	ARG 2			72.113	7.513	-0.474	1.00 32.48 A
55	MOTA	535	N	LEU 2	A	137	73.019	8.329	1.406	1.00 30.72 A
	MOTA	536	CA	LEU 2	A	137	74.371	8.253	0.873	1.00 30.30 A
	MOTA	537	CB	LEU 2			75.167	9.508	1.262	1.00 29.84 A
	ATOM	538	CG	LEU 2			74.541	10.843	0.831	1.00 30.25 A
	ATOM	539		LEU			75.488	11.963	1.154	1.00 29.16 A

	MOTA	540		LEU			74.230	10.835	-0.656	1.00 29.68 A
	MOTA	541	C	LEU			75.083	7.006	1.369	1.00 29.52 A
	MOTA	542	0	LEU	Α	137	75.033	6.684	2.553	1.00 31.12 A
	ATOM	543	N	ASP	Α	138	75.745	6.310	0.453	1.00 27.02 A
5	ATOM	544	CA	ASP	Α	138	76.467	5.087	0.773	1.00 25.70 A
	MOTA	545	CB	ASP	Α	138	75.556	3.887	0.492	1.00 29.85 A
	ATOM	546	CG	ASP	Α	138	76.198	2.567	0.858	1.00 33.94 A
	ATOM	547	OD1	ASP	Α	138	76.815	2.486	1.949	1.00 34.64 A
	ATOM	548	OD2	ASP	Α	138	76.074	1.610	0.058	1.00 35.28 A
10	ATOM	549	C	ASP	А	138	77.699	5.062	-0.127	1.00 24.23 A
	ATOM	550	o	ASP			77,765	4.300	-1.091	1.00 24.33 A
	ATOM	551	N	HIS			78,672	5.904	0.209	1.00 20.89 A
	ATOM	552	CA	HIS		139	79.888	6.069	-0.577	1.00 19.30 A
	ATOM	553	CB	HIS		139	79.681	7.243	-1.553	1.00 17.75 A
15	ATOM	554	CG	HIS		139	80.774	7.410	-2.564	1.00 17.45 A
	ATOM	555		HIS		139	80.794	7.179	-3.897	1.00 16.63 A
	ATOM	556		HIS			82.034	7.862	-2.235	1.00 20.01 A
	ATOM	557		HIS		139	82.784	7.901	-3.322	1.00 20.01 A
	ATOM	558		HIS			82.054	7.491	-4.344	1.00 16.09 A
20	ATOM	559	C	HIS		139	81.066	6.347	0.352	1.00 10.94 A
20	ATOM	560	Ö	HIS			80.914	6.990	1.388	1.00 19.23 A
	MOTA	561	N	PRO		140	82.265	5.881	-0.021	1.00 17.84 A
	MOTA	562	CD	PRO		140	82.575	5.120	-1.243	1.00 16.07 A
2.5	MOTA	563	CA	PRO			83.467	6.079	0.789	1.00 18.04 A
25	MOTA	564	CB	PRO			84.518	5.240	0.055	1.00 18.70 A
	MOTA	565	CG	PRO		140	84.061	5.315	-1.365	1.00 19.17 A
	MOTA	566	С	PRO		140	83.919	7.523	1.014	1.00 19.75 A
	MOTA	567	0	PRO		140	84.686	7.793	1.930	1.00 21.01 A
	MOTA	568	N	PHE			83.460	8.457	0.192	1.00 20.21 A
30	MOTA	569	CA	PHE		141	83.869	9.837	0.389	1.00 20.05 A
	MOTA	570	CB	PHE			84.149	10.496	-0.964	1.00 20.20 A
	MOTA	571	CG	PHE			85.333	9.909	-1.686	1.00 20.95 A
	MOTA	572		PHE			86.362	9.297	-0.975	1.00 21.45 A
	MOTA	573	CD2	PHE		141	85.430	9.983	-3.071	1.00 20.27 A
35	MOTA	574	CE1	PHE			87.476	8.765	-1.635	1.00 22.05 A
	MOTA	575	CE2	PHE			86.541	9.456	-3.743	1.00 20.58 A
	MOTA	576	CZ	PHE	Α	141	87.562	8.848	-3.027	1.00 20.58 A
	MOTA	577	C	PHE	Α	141	82.881	10.679	1.210	1.00 18.71 A
	MOTA	578	0	PHE	Α	141	83.015	11.897	1.300	1.00 19.78 A
40	MOTA	579	N	PHE	Α	142	81.903	10.027	1.823	1.00 18.61 A
	ATOM	580	CA	PHE	Α	142	80.915	10.738	2.639	1.00 19.11 A
	MOTA	581	CB	PHE	Α	142	79.543	10.709	1.966	1.00 17.36 A
	ATOM	582	CG	PHE	Α	142	79.458	11.565	0.750	1.00 19.19 A
	MOTA	583	CD1	PHE	Α	142	79.258	12.936	0.863	1.00 19.44 A
45	ATOM	584	CD2	PHE	Α	142	79.649	11.016	-0.511	1.00 18.39 A
	ATOM	585	CE1	PHE	Α	142	79.254	13.759	-0.268	1.00 20.66 A
	ATOM	586	CE2	PHE	Α	142	79.648	11.824	-1.644	1.00 20.80 A
	ATOM	587	CZ	PHE	Α	142	79.451	13.203	-1.523	1.00 18.95 A
	ATOM	588	С	PHE			80.787	10.132	4.023	1.00 18.98 A
50	ATOM	589	ō	PHE			80.735	8.918	4.168	1.00 18.39 A
	ATOM	590	N	VAL			80.736	10.983	5.041	1.00 20.79 A
	ATOM	591	CA	VAL		143	80.578	10.499	6.401	1.00 20.94 A
	ATOM	592	CB	VAL			80.456	11.670	7.404	1.00 21.95 A
	ATOM	593		VAL		143	80.081	11.145	8.783	1.00 21.30 A
55	ATOM	594		VAL			81.781	12.433	7.473	1.00 21.30 A
55	ATOM	595	C	VAL		143	79.299	9.683	6.396	1.00 19.28 A
	ATOM	596	0	VAL		143	78.280	10.124	5.895	1.00 21.12 A
	ATOM	597	N	LYS		144	79.367	8.481	6.940	1.00 23.63 A
		598	CA	LYS				7.582	6.990	1.00 23.64 A
	MOTA	298	CA	FIS	А	144	78.221	7.582	0.990	1.00 24.4/ A

	MOTA	599	CB	LYS			78.714	6.131		1.00 25.53 A
	MOTA	600	CG	LYS	Α	144	77.635	5.061	6.997	1.00 32.25 A
	MOTA	601	CD	LYS	Α	144	78.240	3.660	6.870	1.00 36.07 A
	ATOM	602	CE	LYS	Α	144	77.187	2.563	7.033	1.00 38.50 A
5	ATOM	603	NZ	LYS	Α	144	77.791	1.186	7.051	1.00 41.46 A
	ATOM	604	C	LYS	А	144	77.418	7.744	8.275	1.00 22.60 A
	ATOM	605	ō	LYS		144	77.973	8.019		1.00 23.18 A
	ATOM	606	N	LEU			76.104	7.583		1.00 21.59 A
	ATOM	607	CA	LEU			75.224	7.661		1.00 21.39 A
10					м					
10	MOTA	608	CB	LEU		145	73.918	8.372		0.50 21.21 AC1
	MOTA	609	CG	LEU		145	72.843			0.50 21.32 AC1
	ATOM	610		LEU		145	73.356			0.50 19.59 AC1
	ATOM	611	CD2	LEU		145	71.569	8.994		0.50 21.45 AC1
	ATOM	612	C	LEU	Α	145	74.919	6.215	9.733	1.00 21.84 A
15	ATOM	613	0	LEU	Α	145	74.283	5.471	8.977	1.00 19.24 A
	ATOM	614	N	TYR	Α	146	75.363	5.816	10.921	1.00 19.77 A
	ATOM	615	CA	TYR	А	146	75.143	4.444	11.368	1.00 19.92 A
	ATOM	616	CB	TYR			76.326	3.944		1.00 18.05 A
	ATOM	617	CG	TYR			77.601	3.803		1.00 17.64 A
20	ATOM	618		TYR			78.435	4.909		1.00 17.04 A
20		619	CE1	TYR			79.638	4.782		1.00 18.26 A
	ATOM									
	ATOM	620	CD2	TYR			78.000	2.560		1.00 15.57 A
	ATOM	621		TYR			79.208	2.419		1.00 17.53 A
	MOTA	622	CZ	TYR			80.022	3.535		1.00 18.78 A
25	ATOM	623	OH	TYR			81.224	3.413		1.00 19.47 A
	MOTA	624	C	TYR			73.884	4.194		1.00 20.60 A
	MOTA	625	0	TYR	Α	146	73.331	3.100	12.108	1.00 21.73 A
	MOTA	626	N	PHE	Α	147	73.431	5.192	12.921	1.00 20.92 A
	ATOM	627	CA	PHE	Α	147	72.239	5.025	13.745	1.00 22.59 A
30	ATOM	628	CB	PHE	А	147	72.538	4.063	14.917	1.00 22.24 A
	ATOM	629	CG	PHE			73.708	4.488		1.00 21.88 A
	ATOM	630		PHE			73.607	5.578		1.00 21.93 A
	ATOM	631	CD2	PHE			74.936	3.843		1.00 21.55 A
	ATOM	632	CE1	PHE			74.715	6.025		1.00 21.37 A
2.5										
35	ATOM	633	CE2	PHE			76.051	4.279		1.00 21.30 A
	ATOM	634	CZ	PHE			75.942	5.371		1.00 24.23 A
	MOTA	635	C	PHE			71.737	6.343		1.00 23.77 A
	MOTA	636	0	PHE			72.448	7.352		1.00 22.91 A
	ATOM	637	N	THR	Α	148	70.501	6.324		1.00 25.15 A
40	MOTA	638	CA	THR	Α	148	69.908	7.503	15.403	1.00 25.99 A
	ATOM	639	CB	THR	Α	148	68.953	8.251	14.466	1.00 27.00 A
	ATOM	640	OG1	THR	Α	148	67.850	7.400	14.148	1.00 27.79 A
	ATOM	641	CG2	THR	Α	148	69.660	8.661	13.193	1.00 26.35 A
	ATOM	642	С	THR			69.080	7.055		1.00 26.23 A
45	ATOM	643	0	THR			68.591	5.930		1.00 26.46 A
	ATOM	644	N	PHE			68.942	7.943		1.00 25.72 A
	ATOM	645	CA	PHE			68.133	7.662	18.706	1.00 25.10 A
	ATOM	646	CB	PHE			68.789	6.593		1.00 23.10 A
	MOTA	647	CG	PHE			70.088	7.011		1.00 22.26 A
50	MOTA	648		PHE			70.105	7.794	21.373	1.00 20.98 A
	MOTA	649	CD2	PHE			71.302	6.587		1.00 21.51 A
	MOTA	650	CE1	PHE			71.312	8.151		1.00 22.36 A
	ATOM	651	CE2	PHE	Α	149	72.511	6.939	20.288	1.00 21.06 A
	ATOM	652	CZ	PHE	Α	149	72.519	7.722	21.430	1.00 19.46 A
55	ATOM	653	C	PHE	Α	149	67.931	8.974	19.427	1.00 27.05 A
	ATOM	654	0	PHE	Α	149	68.565	9.974	19.096	1.00 27.03 A
	ATOM	655	N	GLN		150	67.024	8.984	20.391	1.00 29.18 A
	ATOM	656	CA	GLN			66.757	10.198	21.133	1.00 31.94 A
	ATOM	657	CB	GLN			65.697	11.035		1.00 32.80 A

	ATOM	658	CG	GLN			64.385	10.302	20.153	1.00 34.22 A	
	MOTA	659	CD	GLN	Α	150	63.340	11.169	19.459	1.00 36.88 A	
	MOTA	660	OE1	GLN	Α	150	62.630	11.959	20.098	1.00 37.60 A	
	MOTA	661	NE2	GLN	Α	150	63.248	11.033	18.141	1.00 35.03 A	
5	ATOM	662	C	GLN	Α	150	66.269	9.890	22.531	1.00 32.97 A	
	ATOM	663	0	GLN	А	150	65.857	8.768	22.825	1.00 33.19 A	
	ATOM	664	N	ASP			66.355	10.890	23.398	1.00 34.27 A	
	ATOM	665	CA	ASP			65.847	10.771	24.753	1.00 35.77 A	
	ATOM	666	CB	ASP			66.957	10.933	25.796	1.00 35.66 A	
10	ATOM	667	CG	ASP			67.760	12.194	25.604	1.00 38.11 A	
	ATOM	668		ASP			67.172	13.216	25.195	1.00 39.31 A	
	ATOM	669		ASP			68.982	12.167	25.879	1.00 39.31 A	
	ATOM	670	C	ASP			64.823	11.904	24.838		
	ATOM	671	0	ASP			64.401	12.428	23.803		
15	MOTA	672	N	ASP			64.427	12.301	26.041	1.00 38.18 A	
	MOTA	673	CA	ASP			63.427	13.357	26.171	1.00 39.81 A	
	MOTA	674	CB	ASP			63.022	13.534	27.637	1.00 44.46 A	
	MOTA	675	CG	ASP			62.291	12.324	28.186	1.00 50.02 A	
	MOTA	676		ASP			61.313	11.876	27.541	1.00 52.36 A	
20	MOTA	677		ASP			62.689	11.822	29.263	1.00 52.75 A	
	ATOM	678	C	ASP			63.822	14.709	25.594	1.00 37.45 A	
	ATOM	679	0	ASP	Α	152	62.988	15.408	25.026	1.00 36.81 A	
	ATOM	680	N	GLU	Α	153	65.091	15.077	25.708	1.00 35.46 A	
	ATOM	681	CA	GLU	Α	153	65.501	16.378	25.211	1.00 33.50 A	
25	ATOM	682	CB	GLU	Α	153	66.132	17.174	26.354	1.00 36.16 A	
	ATOM	683	CG	GLU	Α	153	65.389	17.065	27.687	1.00 37.72 A	
	ATOM	684	CD	GLU	А	153	65.657	15.753	28.402	0.00 37.23 A	
	ATOM	685	OE1	GLU	А	153	65.063	15.530	29.479	0.00 37.39 A	
	ATOM	686	OE2	GLU	А	153	66.464	14.947	27.893	0.00 37.39 A	
30	ATOM	687	C	GLU			66.432	16.425	23.995	1.00 31.79 A	
	ATOM	688	Ö	GLU			66.498	17.451	23.323	1.00 30.80 A	
	ATOM	689	N	LYS			67.131	15.334	23.691	1.00 30.35 A	
	ATOM	690	CA	LYS			68.069	15.357	22.569	1.00 28.14 A	
	ATOM	691	CB	LYS			69.505	15.358	23.099	1.00 27.32 A	
35	ATOM	692	CG	LYS			69.853	16.503	24.026	1.00 29.91 A	
33	ATOM	693	CD	LYS			71.234	16.302	24.648	1.00 29.91 A	
	ATOM	694	CE	LYS			71.606	17.450	25.592	1.00 30.14 A	
	MOTA	695	NZ	LYS			72.780	17.121	26.469	1.00 31.90 A	
40	MOTA	696	C	LYS			67.967	14.261	21.515	1.00 26.36 A	
40	MOTA	697	0	LYS			67.517	13.145	21.781	1.00 23.71 A	
	MOTA	698	N	LEU			68.413	14.610	20.311	1.00 24.76 A	
	MOTA	699	CA	LEU			68.462	13.691	19.178	1.00 23.29 A	
	ATOM	700	CB	LEU			68.012	14.382	17.891	1.00 22.72 A	
	MOTA	701	CG	LEU			66.588	14.916	17.739	1.00 24.25 A	
45	ATOM	702		LEU			66.441	15.489	16.329	1.00 24.62 A	
	MOTA	703	CD2	LEU			65.576	13.798	17.965	1.00 23.10 A	
	ATOM	704	С	LEU	Α	155	69.939	13.325	19.022	1.00 21.93 A	
	ATOM	705	0	LEU	Α	155	70.812	14.167	19.233	1.00 20.17 A	
	MOTA	706	N	TYR	Α	156	70.227	12.088	18.647	1.00 19.72 A	
50	ATOM	707	CA	TYR	Α	156	71.617	11.693	18.462	1.00 20.11 A	
	ATOM	708	CB	TYR	А	156	72.061	10.703	19.540	1.00 20.01 A	
	ATOM	709	CG	TYR			71.885	11.172	20.963	1.00 20.98 A	
	ATOM	710		TYR			70.619	11.313	21.520	1.00 22.18 A	
	ATOM	711	CE1	TYR		156	70.457	11.724	22.850	1.00 25.21 A	
55	ATOM	712	CD2	TYR			72.991	11.449	21.762	1.00 21.38 A	
	ATOM	713	CE2	TYR			72.843	11.859	23.086	1.00 25.12 A	
	ATOM	714	CZ	TYR			71.576	11.995	23.622	1.00 24.83 A	
	ATOM	715	OH	TYR			71.431	12.410	24.923	1.00 24.03 A	
	ATOM	716	C	TYR			71.792	11.033	17.108	1.00 20.02 A	
	AIUH	1.10	-	TIK	м	170	11.152	TT.003	T/.TU0	1.00 ZU.UZ A	

	ATOM	717	0	TYR			70.959	10.231	16.704	1.00 22.19 A
	MOTA	718	N	PHE			72.860	11.385	16.399	1.00 19.17 A
	ATOM	719	CA	PHE	Α	157	73.140	10.769	15.114	1.00 18.65 A
	ATOM	720	CB	PHE	Α	157	73.071	11.780	13.969	1.00 21.02 A
5	ATOM	721	CG	PHE	Α	157	71.719	12.411	13.791	1.00 25.64 A
	MOTA	722	CD1	PHE	А	157	70.558	11.724	14.135	1.00 27.84 A
	ATOM	723	CD2	PHE		157	71,603	13.695	13.267	1.00 27.19 A
	ATOM	724		PHE			69.301	12.310	13.964	1.00 28.87 A
	ATOM	725	CE2	PHE			70.350	14.288	13.091	1.00 28.27 A
10		726		PHE			69.200	13.595	13.442	
10	ATOM		CZ							
	MOTA	727	С	PHE			74.543	10.212	15.204	1.00 19.60 A
	MOTA	728	0	PHE			75.489	10.952	15.467	1.00 19.26 A
	MOTA	729	N	GLY			74.668	8.902	15.010	1.00 19.26 A
	MOTA	730	CA	GLY	Α	158	75.972	8.265	15.063	1.00 18.63 A
15	ATOM	731	C	GLY	Α	158	76.615	8.309	13.693	1.00 16.84 A
	ATOM	732	0	GLY	Α	158	76.160	7.646	12.772	1.00 15.29 A
	ATOM	733	N	LEU	А	159	77.677	9.096	13.567	1.00 18.10 A
	ATOM	734	CA	LEU			78.386	9.263	12.302	1.00 17.32 A
	ATOM	735	CB	LEU			78.502	10.753	11.984	1.00 16.80 A
20	ATOM	736	CG	LEU			77.161	11.485	12.068	1.00 18.21 A
20	ATOM	737		LEU			77.376	12.992	12.058	1.00 15.34 A
	ATOM	738		LEU			76.280	11.036	10.906	1.00 13.34 A
	MOTA	739	C	LEU			79.780	8.665	12.375	1.00 18.27 A
	MOTA	740	0	LEU			80.338	8.518	13.465	1.00 18.92 A
25	MOTA	741	N	SER			80.343	8.320	11.220	1.00 16.88 A
	MOTA	742	CA	SER			81.691	7.770	11.194	1.00 19.02 A
	MOTA	743	CB	SER			82.086	7.362	9.771	1.00 20.02 A
	MOTA	744	OG	SER			81.866	8.421	8.864	1.00 25.88 A
	ATOM	745	C	SER	Α	160	82.655	8.831	11.724	1.00 18.34 A
30	MOTA	746	0	SER	Α	160	82.413	10.032	11.588	1.00 17.84 A
	ATOM	747	N	TYR	Α	161	83.743	8.384	12.335	1.00 17.11 A
	ATOM	748	CA	TYR	Α	161	84.723	9.300	12.901	1.00 19.21 A
	ATOM	749	CB	TYR	А	161	85.146	8.802	14.293	1.00 19.37 A
	ATOM	750	CG	TYR	А	161	86.269	9.582	14.944	1.00 22.52 A
35	ATOM	751		TYR			86.276	10.978	14.929	1.00 21.17 A
	ATOM	752	CE1	TYR			87.283	11.703	15.559	1.00 18.10 A
	ATOM	753	CD2	TYR			87.313	8.923	15.612	1.00 21.92 A
	ATOM	754	CE2	TYR			88.330	9.647	16.252	1.00 20.10 A
	ATOM	755	CZ	TYR			88.301	11.039	16.232	1.00 20.10 A
40										
40	ATOM	756	OH	TYR			89.266	11.776	16.873	1.00 20.31 A
	MOTA	757	C	TYR			85.934	9.459	11.997	1.00 20.13 A
	MOTA	758	0	TYR			86.621	8.491	11.675	1.00 21.97 A
	MOTA	759	N	ALA			86.182	10.686	11.571	1.00 19.13 A
	MOTA	760	CA	ALA			87.320	10.969	10.717	1.00 20.60 A
45	MOTA	761	CB	ALA	Α	162	86.907	11.919	9.592	1.00 21.18 A
	MOTA	762	C	ALA	Α	162	88.375	11.617	11.604	1.00 21.36 A
	ATOM	763	0	ALA	Α	162	88.391	12.835	11.752	1.00 20.74 A
	ATOM	764	N	LYS	Α	163	89.237	10.787	12.195	1.00 21.80 A
	MOTA	765	CA	LYS			90.294	11.232	13.102	1.00 25.38 A
50	ATOM	766	CB	LYS			91.315	10.109	13.332	1.00 30.51 A
	ATOM	767	CG	LYS			90.874	8.987	14.251	1.00 38.24 A
	ATOM	768	CD	LYS			92.000	7.970	14.456	1.00 43.14 A
	ATOM	769	CE	LYS			91.556	6.794	15.342	1.00 45.14 A
	ATOM	770	NZ	LYS			91.252	7.200	16.752	1.00 48.83 A
55										
23	ATOM	771	C	LYS			91.082	12.482	12.719	1.00 25.07 A
	MOTA	772	0	LYS			91.276	13.373	13.541	1.00 25.50 A
	ATOM	773	N	ASN		164	91.540	12.549	11.477	1.00 25.06 A
	MOTA	774	CA	ASN			92.363	13.668	11.054	1.00 26.04 A
	MOTA	775	CB	ASN	Α	164	93.115	13.278	9.787	1.00 26.02 A

	ATOM	776	CG	ASN A	164	94.062	12.120	10.033	1.00 29.07 A
	ATOM	777		ASN A		94.854	12.155	10.969	1.00 30.18 A
	ATOM	778		ASN A		93.979	11.089	9.207	1.00 32.14 A
	MOTA	779	C	ASN A		91.725	15.040	10.915	1.00 25.35 A
5	ATOM	780	0	ASN A		92.416	16.021	10.640	1.00 26.51 A
	MOTA	781	N	GLY A	165	90.419	15.122	11.116	1.00 23.92 A
	ATOM	782	CA	GLY A	165	89.761	16.413	11.043	1.00 24.35 A
	ATOM	783	C	GLY A		89.663	17.123	9.704	1.00 23.94 A
	ATOM	784	o	GLY A		89.632	16.501	8.643	1.00 25.49 A
10									
10		785	N	GLU A		89.623	18.449	9.773	1.00 23.07 A
	ATOM	786	CA	GLU A		89.467	19.301	8.602	1.00 23.26 A
	MOTA	787	CB	GLU A	166	89.164	20.739	9.036	1.00 23.73 A
	ATOM	788	CG	GLU A	166	88.271	20.875	10.257	1.00 27.31 A
	ATOM	789	CD	GLU A		87.812	22.302	10.474	1.00 29.74 A
15		790		GLU A		88.586	23.221	10.130	1.00 30.87 A
13									
	MOTA	791		GLU A		86.686	22.510	10.989	1.00 29.80 A
	ATOM	792	С	GLU A		90.612	19.354	7.602	1.00 24.47 A
	MOTA	793	0	GLU A	166	91.786	19.473	7.968	1.00 24.85 A
	ATOM	794	N	LEU A	167	90.251	19.287	6.328	1.00 23.47 A
20		795	CA	LEU A		91.228	19.393	5.262	1.00 24.00 A
20	ATOM	796	CB	LEU A		90.528	19.369	3.901	1.00 22.48 A
	MOTA	797	CG	LEU A		91.373	19.759	2.679	1.00 23.87 A
	MOTA	798		LEU A		92.583	18.846	2.563	1.00 20.03 A
	MOTA	799	CD2	LEU A	167	90.516	19.680	1.418	1.00 22.08 A
25	ATOM	800	C	LEU A	167	91.943	20.732	5.448	1.00 24.82 A
	ATOM	801	0	LEU A	167	93.138	20.858	5.165	1.00 24.59 A
	ATOM	802	N	LEU A		91.206	21.731	5.927	1.00 24.43 A
	ATOM	803	CA	LEU A		91.784	23.055	6.150	1.00 24.45 A
	MOTA	804	CB	LEU A		90.746	24.009	6.747	1.00 27.44 A
30		805	CG	LEU A		91.310	25.395	7.090	1.00 28.57 A
	MOTA	806	CD1	LEU A	168	91.624	26.150	5.809	1.00 28.11 A
	ATOM	807	CD2	LEU A	168	90.312	26.174	7.921	1.00 29.97 A
	ATOM	808	C	LEU A		92.999	23.014	7.074	1.00 28.43 A
	ATOM	809	ō	LEU A		93.952	23.760	6.882	1.00 30.21 A
35		810	N	LYS A		92.958	22.152	8.081	1.00 30.21 A
33									
	MOTA	811	CA	LYS A		94.072	22.050	9.008	1.00 33.52 A
	MOTA	812	CB	LYS A		93.821	20.955	10.046	1.00 35.45 A
	MOTA	813	CG	LYS A	169	94.972	20.784	11.033	1.00 40.43 A
	ATOM	814	CD	LYS A	169	94.808	19.562	11.943	1.00 41.43 A
40		815	CE	LYS A		95.047	18.261	11.186	1.00 42.67 A
	ATOM	816	NZ	LYS A		95.057	17.068	12.096	1.00 43.84 A
			c	LYS A		95.329			
	MOTA	817					21.718	8.228	
	MOTA	818	0	LYS A		96.377	22.333	8.421	1.00 35.58 A
	MOTA	819	N	TYR A		95.219	20.739	7.339	1.00 34.55 A
45	MOTA	820	CA	TYR A	170	96.357	20.328	6.539	1.00 35.07 A
	ATOM	821	CB	TYR A	170	96.018	19.047	5.790	1.00 35.72 A
	ATOM	822	CG	TYR A	170	96.050	17.869	6.716	1.00 37.48 A
	ATOM	823		TYR A		97.256	17.250	7.040	1.00 39.42 A
		824		TYR A			16.230	7.987	1.00 40.93 A
50	ATOM					97.313			
50		825		TYR A		94.895	17.435	7.355	1.00 38.83 A
	MOTA	826	CE2	TYR A	170	94.937	16.417	8.303	1.00 41.76 A
	ATOM	827	CZ	TYR A	170	96.149	15.821	8.615	1.00 42.18 A
	ATOM	828	OH	TYR A	170	96.196	14.827	9.563	1.00 45.30 A
	ATOM	829	C	TYR A		96.823	21.404	5.585	1.00 35.67 A
55		830	ō	TYR A		97.999	21.465	5.248	1.00 35.28 A
33									
	MOTA	831	N	ILE A		95.904	22.260	5.154	1.00 36.78 A
	MOTA	832	CA	ILE A		96.272	23.333	4.252	1.00 38.95 A
	ATOM	833	CB	ILE A		95.032	24.048	3.682	1.00 39.15 A
	MOTA	834	CG2	ILE A	171	95.452	25.329	2.960	1.00 38.11 A

	ATOM	835		ILE			94.296	23.113	2.718	1.00 37.57 A
	MOTA	836	CD1	ILE			93.041	23.712	2.116	1.00 37.48 A
	ATOM	837	C	ILE			97.146	24.338	4.990	1.00 41.33 A
	ATOM	838	0	ILE		171	98.173	24.765	4.466	1.00 42.36 A
5	ATOM	839	N	ARG	Α	172	96.748	24.713	6.203	1.00 42.79 A
	MOTA	840	CA	ARG	Α	172	97.541	25.662	6.981	1.00 44.62 A
	ATOM	841	CB	ARG	Α	172	96.809	26.103	8.253	1.00 46.82 A
	MOTA	842	CG	ARG	Α	172	95.492	26.828	8.033	1.00 50.73 A
	MOTA	843	CD	ARG	Α	172	95.124	27.643	9.271	1.00 53.80 A
10	MOTA	844	NE	ARG	Α	172	93.747	28.136	9.247	1.00 56.88 A
	ATOM	845	CZ	ARG	А	172	93.183	28.766	8.218	1.00 57.65 A
	ATOM	846		ARG		172	93.873	28.989	7.104	1.00 57.71 A
	ATOM	847		ARG			91.923	29.176	8.305	1.00 56.95 A
	ATOM	848	С	ARG			98.856	25.015	7.383	1.00 44.41 A
15	ATOM	849	ō	ARG			99.927	25.587	7.186	1.00 45.16 A
	ATOM	850	N	LYS		173	98.759	23.817	7.949	1.00 44.01 A
	ATOM	851	CA	LYS			99.923	23.069	8.398	1.00 42.99 A
	ATOM	852	CB	LYS		173	99.538	21.616	8.667	1.00 44.20 A
	ATOM	853	CG	LYS		173	100.721	20.689	8.908	1.00 45.81 A
20	ATOM	854	CD	LYS		173	100.721	19.238	8.987	0.00 45.28 A
20	ATOM	855	CE	LYS		173	101.457	18.296	9.120	0.00 45.28 A
	ATOM	856	NZ	LYS		173	101.437			0.00 45.45 A
								16.870	9.146	
	MOTA	857	С	LYS		173	101.081	23.108	7.412	1.00 43.20 A
2.5	ATOM	858	0	LYS		173	102.220	23.366	7.805	1.00 43.49 A
25	ATOM	859	N	ILE		174	100.802	22.867	6.133	1.00 41.97 A
	ATOM	860	CA	ILE		174	101.871	22.859	5.136	1.00 40.74 A
	MOTA	861	CB	ILE		174	101.874	21.536	4.336	1.00 40.61 A
	MOTA	862	CG2	ILE		174	101.897	20.352	5.297	1.00 41.39 A
	MOTA	863		ILE		174	100.638	21.448	3.442	1.00 40.75 A
30	MOTA	864	CD1	ILE		174	100.680	20.276	2.487	1.00 40.45 A
	MOTA	865	C	ILE		174	101.882	24.024	4.149	1.00 39.97 A
	ATOM	866	0	ILE		174	102.675	24.033	3.209	1.00 38.15 A
	MOTA	867	N	GLY			101.007	25.004	4.359	1.00 40.09 A
	MOTA	868	CA	GLY		175	100.969	26.156	3.473	1.00 39.94 A
35	ATOM	869	C	GLY	Α	175	100.151	25.960	2.211	1.00 39.87 A
	ATOM	870	0	GLY	Α	175	99.152	26.646	2.005	1.00 40.53 A
	MOTA	871	N	SER	Α	176	100.586	25.043	1.354	1.00 39.28 A
	MOTA	872	CA	SER			99.871	24.747	0.122	1.00 38.77 A
	MOTA	873	CB	SER	Α	176	100.169	25.804	-0.950	1.00 39.84 A
40	MOTA	874	OG	SER	Α	176	101.537	25.823	-1.319	1.00 43.67 A
	ATOM	875	C	SER	Α	176	100.265	23.353	-0.358	1.00 38.39 A
	ATOM	876	0	SER	Α	176	101.245	22.776	0.118	1.00 39.37 A
	ATOM	877	N	PHE	Α	177	99.491	22.811	-1.289	1.00 35.85 A
	ATOM	878	CA	PHE	Α	177	99.732	21.472	-1.810	1.00 32.81 A
45	ATOM	879	CB	PHE	А	177	98.401	20.770	-2.095	1.00 32.30 A
	ATOM	880	CG	PHE		177	97.645	20.344	-0.867	1.00 31.20 A
	ATOM	881		PHE		177	97.806	21.005	0.348	1.00 29.02 A
	ATOM	882	CD2	PHE		177	96.735	19.293	-0.939	1.00 30.11 A
	ATOM	883		PHE		177	97.076	20.628	1.468	1.00 27.07 A
50	ATOM	884	CE2	PHE		177	95.998	18.910	0.181	1.00 29.70 A
50	ATOM	885	CZ	PHE			96.170	19.580	1.385	1.00 27.57 A
	ATOM	886	C	PHE		177	100.535	21.485	-3.093	1.00 27.37 A
	ATOM	887	0	PHE		177	100.335	22.381	-3.093	1.00 33.02 A
	ATOM	888	N			178	100.386	20.471	-3.927	1.00 30.75 A
55		889		ASP		178	102.184	20.471		
23	ATOM		CA						-4.454	
	ATOM	890	CB	ASP		178	103.269	19.275	-4.244	1.00 35.60 A
	MOTA	891	CG	ASP		178	102.693	17.932	-3.855	1.00 40.22 A
	MOTA	892		ASP		178	101.840	17.412	-4.612	1.00 42.64 A
	MOTA	893	OD2	ASP	Α	178	103.079	17.398	-2.793	1.00 43.32 A

	MOTA	894	C	ASP A 1		101.195	19.859	-5.519		32.50	
	ATOM	895	0	ASP A 1	78	99.999	19.723	-5.245	1.00	30.51	Α
	ATOM	896	N	GLU A 1	79	101.684	19.584	-6.720	1.00	31.46	Α
	ATOM	897	CA	GLU A 1	79	100.790	19.160	-7.779		32.00	
	5 ATOM	898	CB	GLU A 1	79	101.480	19.291	-9.138	1.00	33.70	A
	ATOM	899	CG	GLU A 1	79	100.666	18.711	-10.284	1.00	38.81	A
	ATOM	900	CD	GLU A 1	79	101.129	19.195	-11.646	1.00	42.71	A
	ATOM	901	OE1	GLU A 1	79	102.358	19.338	-11.844	1.00	43.96	Α
	ATOM	902	OE2	GLU A 1	79	100.261	19.422	-12.523	1.00	44.44	Α
1	MOTA 0	903	C	GLU A 1	79	100.189	17.766	-7.635	1.00	29.96	Α
	ATOM	904	0	GLU A 1	79	99.023	17.564	-7.965	1.00	27.38	Α
	ATOM	905	N	THR A 1	80	100.959	16.803	-7.141	1.00	30.09	Α
	ATOM	906	CA	THR A 1	80	100.429	15.448	-7.007	1.00	29.75	Α
	ATOM	907	CB	THR A 1	80	101.583	14.416	-6.738	1.00	30.62	А
1	5 ATOM	908	OG1	THR A 1	80	101.050	13.206	-6.179	1.00	30.65	Α
	ATOM	909	CG2	THR A 1	80	102.615	14.991	-5.802	1.00	32.90	Α
	ATOM	910	C	THR A 1	80	99.331	15.372	-5.935	1.00	29.43	Α
	ATOM	911	0	THR A 1	80	98.312	14.710	-6.130	1.00	27.52	А
	ATOM	912	N	CYS A 1	81	99.522	16.079	-4.823	1.00	29.55	Α
2		913	CA	CYS A 1	81	98.535	16.091	-3.745	1.00	29.27	Α
	ATOM	914	CB	CYS A 1	81	99.156	16.681	-2.480	1.00	31.47	А
	ATOM	915	SG	CYS A 1	81	100.580	15.747	-1.838	1.00	39.84	Α
	ATOM	916	С	CYS A 1		97.271	16.879	-4.126	1.00	28.16	А
	ATOM	917	0	CYS A 1	81	96.156	16.495	-3.762	1.00	26.55	Α
2	5 ATOM	918	N	THR A 1	82	97.441	17.984	-4.847	1.00	25.71	A
	ATOM	919	CA	THR A 1	82	96.293	18.784	-5.268	1.00	24.22	Α
	ATOM	920	CB	THR A 1	82	96.714	20.043	-6.066	1.00	24.45	Α
	ATOM	921	OG1	THR A 1	82	97.515	20.901	-5.241	1.00	22.57	Α
	ATOM	922	CG2	THR A 1	82	95.483	20.809	-6.537	1.00	23.42	Α
3	MOTA 0	923	С	THR A 1	82	95.447	17.915	-6.184	1.00	24.78	A
	ATOM	924	0	THR A 1	82	94.227	17.812	-6.020	1.00	23.72	A
	ATOM	925	N	ARG A 1	83	96.109	17.283	-7.149	1.00	23.96	Α
	MOTA	926	CA	ARG A 1	83	95.422	16.419	-8.096	1.00	25.38	A
	MOTA	927	CB	ARG A 1		96.416	15.782	-9.073			A
3	5 ATOM	928	CG	ARG A 1	83	95.740		-10.044		27.88	
	MOTA	929	CD	ARG A 1	83	96.704	14.244	-11.070	1.00	30.56	Α
	MOTA	930	NE	ARG A 1	83	97.260		-11.904	1.00	34.63	A
	MOTA	931	CZ	ARG A 1		98.502	15.756	-11.802		33.50	
	ATOM	932		ARG A 1		99.328		-10.903		31.79	A
4	MOTA 0	933	NH2	ARG A 1	83	98.901		-12.579			A
	MOTA	934	C	ARG A 1		94.648	15.318	-7.386			Α
	ATOM	935	0	ARG A 1		93.466	15.099	-7.659			A
	ATOM	936	N	PHE A 1		95.319	14.628	-6.473		23.84	
	ATOM	937	CA	PHE A 1		94.689	13.541	-5.742		23.63	
4		938	CB	PHE A 1		95.662	12.941	-4.730		25.29	A
	MOTA	939	CG	PHE A 1		95.086	11.787	-3.961			Α
	ATOM	940		PHE A 1		94.958	10.531	-4.556		30.34	
	ATOM	941	CD2	PHE A 1		94.620	11.964	-2.663			A
	ATOM	942		PHE A 1		94.370	9.465	-3.871			A
5		943	CE2	PHE A 1		94.030	10.908	-1.969			A
	MOTA	944	CZ	PHE A 1		93.904	9.654	-2.576		29.09	
	MOTA	945	C	PHE A 1		93.431	13.977	-5.003		23.55	
	ATOM	946	0	PHE A 1		92.353	13.429	-5.219		24.05	
_	MOTA	947	N	TYR A 1		93.568	14.961	-4.124			A
5		948	CA	TYR A 1		92.429	15.408	-3.344		21.69	
	MOTA	949	CB	TYR A 1		92.925	16.295	-2.200		22.66	
	MOTA	950	CG	TYR A 1		93.539	15.447	-1.097			A
	MOTA	951		TYR A 1		92.738	14.614	-0.314		26.51	
	ATOM	952	CE1	TYR A 1	85	93.290	13.738	0.620	1.00	27.53	A

	ATOM	953		TYR			94.924	15.391	-0.908	1.00 28.66 A
	ATOM	954	CE2	TYR			95.496	14.514	0.032	1.00 29.09 A
	MOTA	955	CZ	TYR			94.667	13.688	0.790	1.00 29.75 A
	ATOM	956	OH	TYR	Α	185	95.204	12.806	1.702	1.00 29.03 A
5	ATOM	957	C	TYR	Α	185	91.316	16.058	-4.167	1.00 21.02 A
	MOTA	958	0	TYR	Α	185	90.130	15.921	-3.851	1.00 18.76 A
	ATOM	959	N	THR	Α	186	91.689	16.731	-5.244	1.00 19.87 A
	ATOM	960	CA	THR	Α	186	90.690	17.337	-6.102	1.00 18.89 A
	ATOM	961	CB	THR			91.344	18.170	-7.200	1.00 19.73 A
10	ATOM	962		THR		186	92.115	19.218	-6.603	1.00 19.38 A
	ATOM	963		THR			90.282	18.765	-8.125	1.00 20.16 A
	ATOM	964	C	THR			89.905	16.201	-6.753	1.00 19.05 A
	ATOM	965	ō	THR			88.675	16.244	-6.855	1.00 19.38 A
	ATOM	966	N	ALA		187	90.627	15.180	-7.200	1.00 18.33 A
15	ATOM	967	CA	ALA			89.984	14.043	-7.841	1.00 18.09 A
15	ATOM	968	CB	ALA			91.024	13.035	-8.276	1.00 19.99 A
	ATOM	969	С	ALA			88.986	13.402	-6.886	1.00 18.07 A
		970		ALA				13.402	-7.291	
	ATOM	970	0	GLU			87.873 89.366	13.055	-5.617	1.00 18.54 A 1.00 16.56 A
20	ATOM		N							
20	MOTA	972	CA	GLU			88.446	12.660	-4.653	1.00 16.18 A
	MOTA	973	CB	GLU		188	89.099	12.495	-3.280	1.00 15.52 A
	MOTA	974	CG	GLU		188	90.266	11.519	-3.259	1.00 20.99 A
	MOTA	975	CD	GLU			90.297	10.636	-2.013	1.00 22.64 A
	MOTA	976		GLU			90.006	11.126	-0.899	1.00 22.95 A
25	MOTA	977	OE2	GLU			90.629	9.439	-2.149	1.00 27.37 A
	MOTA	978	C	GLU		188	87.189	13.508	-4.518	1.00 15.81 A
	MOTA	979	0	GLU			86.080	12.978	-4.460	1.00 15.92 A
	MOTA	980	N	ILE		189	87.364	14.825	-4.483	1.00 16.14 A
	MOTA	981	CA	ILE			86.235	15.733	-4.346	1.00 16.66 A
30	MOTA	982	CB	ILE		189	86.698	17.179	-4.083	1.00 16.57 A
	MOTA	983	CG2	ILE	Α	189	85.485	18.098	-3.958	1.00 14.92 A
	ATOM	984	CG1	ILE	Α	189	87.502	17.235	-2.784	1.00 16.19 A
	MOTA	985	CD1	ILE	Α	189	88.202	18.559	-2.547	1.00 16.78 A
	ATOM	986	C	ILE	Α	189	85.349	15.712	-5.580	1.00 16.29 A
35	ATOM	987	0	ILE	Α	189	84.123	15.667	-5.471	1.00 15.80 A
	ATOM	988	N	VAL	Α	190	85.962	15.743	-6.755	1.00 16.44 A
	ATOM	989	CA	VAL	Α	190	85.186	15.704	-7.985	1.00 15.98 A
	ATOM	990	CB	VAL	Α	190	86.101	15.692	-9.229	1.00 17.23 A
	ATOM	991	CG1	VAL	Α	190	85.280	15.380	-10.488	1.00 16.01 A
40	ATOM	992	CG2	VAL	Α	190	86.797	17.034	-9.373	1.00 13.82 A
	ATOM	993	С	VAL	А	190	84.351	14.433	-7.979	1.00 16.29 A
	ATOM	994	0	VAL	Α	190	83.140	14.462	-8.194	1.00 15.64 A
	ATOM	995	N	SER	А	191	85.011	13.312	-7.723	1.00 18.94 A
	ATOM	996	CA	SER			84.337	12.015	-7.692	1.00 18.50 A
45	ATOM	997	CB	SER			85.357	10.914	-7.427	1.00 19.04 A
	ATOM	998	OG	SER			84.712	9.680	-7.206	1.00 23.87 A
	ATOM	999	C	SER			83.233	11.961	-6.642	1.00 16.85 A
	ATOM	1000	ō	SER			82.227	11.281	-6.818	1.00 18.11 A
	ATOM	1001	N	ALA			83.419	12.671	-5.540	1.00 17.37 A
50	ATOM	1002	CA	ALA			82.395	12.687	-4.501	1.00 17.10 A
50		1002	CB	ALA			82.947	13.302	-3.222	1.00 17.10 A
	ATOM ATOM	1003	CB	ALA			81.218	13.502	-5.020	
				ALA						
	ATOM	1005	0				80.055	13.162	-4.798	1.00 18.91 A
	ATOM	1006	N	LEU			81.524	14.597	-5.725	1.00 16.53 A
55	ATOM	1007	CA	LEU			80.483	15.453	-6.270	1.00 17.25 A
	MOTA	1008	CB	LEU		193	81.091	16.750	-6.826	1.00 17.70 A
	ATOM	1009	CG	LEU		193	81.537	17.738	-5.732	1.00 22.88 A
	ATOM	1010		LEU		193	82.094	19.018	-6.348	1.00 22.13 A
	MOTA	1011	CD2	LEU	Α	193	80.345	18.057	-4.839	1.00 20.04 A

	MOTA	1012	C	LEU A		79.664	14.737	-7.343	1.00 17.26 A
	MOTA	1013	0	LEU A		78.442	14.893	-7.402	1.00 15.43 A
	MOTA	1014	N	GLU A		80.330	13.962	-8.195	1.00 16.22 A
	MOTA	1015	CA	GLU A		79.612	13.232	-9.225	1.00 19.22 A
5	ATOM	1016	CB	GLU A		80.564		-10.086	1.00 20.77 A
	MOTA	1017	CG	GLU A		79.828		-10.978	1.00 26.27 A
	ATOM	1018	CD	GLU A		80.756		-11.934	1.00 29.43 A
	ATOM	1019		GLU A		81.840		-11.489	1.00 28.21 A
	MOTA	1020		GLU A		80.392		-13.127	1.00 31.66 A
10	MOTA	1021	C	GLU A	194	78.599	12.303	-8.566	1.00 19.71 A
	MOTA	1022	0	GLU A	194	77.466	12.159	-9.027	1.00 18.40 A
	ATOM	1023	N	TYR A	195	79.012	11.672	-7.479	1.00 19.22 A
	MOTA	1024	CA	TYR A	195	78.116	10.773	-6.781	1.00 19.69 A
	ATOM	1025	CB	TYR A	195	78.867	10.041	-5.667	1.00 21.39 A
15	ATOM	1026	CG	TYR A	195	77.975	9.143	-4.847	1.00 22.55 A
	ATOM	1027	CD1	TYR A	195	77.596	7.881	-5.316	1.00 23.14 A
	ATOM	1028	CE1	TYR A	195	76.743	7.065	-4.577	1.00 22.98 A
	ATOM	1029		TYR A		77.479	9.564	-3.618	1.00 21.58 A
	ATOM	1030		TYR A		76.625	8.755	-2.872	1.00 23.50 A
20	ATOM	1031	CZ	TYR A		76.263	7.512	-3.358	1.00 23.18 A
	ATOM	1032	OH	TYR A		75.413	6.732	-2.632	1.00 24.19 A
	ATOM	1033	C	TYR A		76.939	11.546	-6.172	1.00 18.80 A
	ATOM	1034	ō	TYR A		75.782	11.164	-6.337	1.00 19.89 A
	ATOM	1035	N	LEU A		77.242	12.629	-5.469	1.00 15.26 A
25	ATOM	1036	CA	LEU A		76.210	13.430	-4.813	1.00 16.52 A
23	ATOM	1037	CB	LEU A		76.855	14.586	-4.038	1.00 15.67 A
	ATOM	1038	CG	LEU A		75.923	15.401	-3.131	1.00 19.13 A
	ATOM	1039		LEU A		75.555	14.571	-1.903	1.00 18.42 A
	ATOM	1040		LEU A		76.604	16.681	-2.689	1.00 18.50 A
30	ATOM	1040	C D Z	LEU A		75.209	13.993	-5.814	1.00 18.30 A
30	ATOM	1041	Ö	LEU A		73.990	13.892	-5.637	1.00 16.12 A
		1042	N	HIS A		75.732	14.592	-6.875	1.00 16.25 A
	ATOM								
	ATOM	1044	CA	HIS A		74.873	15.171	-7.878	1.00 20.69 A
25	ATOM	1045		HIS A		75.715	16.004	-8.832	1.00 19.71 A
35	ATOM	1046	CG	HIS A		76.292	17.224	-8.190	1.00 19.55 A
	ATOM	1047		HIS A		76.069	17.777	-6.973	1.00 18.32 A
	ATOM	1048		HIS A		77.172	18.063	-8.837	1.00 20.26 A
	ATOM	1049		HIS A		77.463	19.084	-8.049	1.00 20.73 A
40	ATOM	1050		HIS A		76.806	18.935	-6.913	1.00 19.92 A
40	ATOM	1051	С	HIS A		74.091	14.093	-8.609	1.00 22.80 A
	ATOM	1052	0	HIS A		72.974	14.328	-9.068	1.00 21.91 A
	ATOM	1053	N	GLY A		74.672	12.903	-8.697	1.00 23.17 A
	ATOM	1054	CA	GLY A		73.990	11.815	-9.366	1.00 26.22 A
45	ATOM	1055	C	GLY A		72.718	11.436	-8.631	1.00 27.16 A
45	MOTA	1056	0	GLY A		71.837	10.787	-9.185	1.00 27.89 A
	MOTA	1057	N	LYS A		72.623	11.831	-7.369	1.00 27.84 A
	MOTA	1058	CA	LYS A		71.429	11.532	-6.587	1.00 28.20 A
	MOTA	1059	CB	LYS A		71.827	10.952	-5.227	1.00 29.35 A
	MOTA	1060	CG	LYS A		72.278	9.502	-5.321	1.00 32.74 A
50	MOTA	1061	CD	LYS A		72.737	8.944	-3.990	1.00 38.22 A
	MOTA	1062	CE	LYS A		72.600	7.424	-3.965	1.00 41.17 A
	MOTA	1063	NZ	LYS A		73.173	6.779	-5.185	1.00 44.70 A
	MOTA	1064	C	LYS A		70.542	12.765	-6.419	1.00 26.97 A
	MOTA	1065	0	LYS A		69.678	12.807	-5.551	1.00 28.27 A
55	MOTA	1066	N	GLY A		70.759	13.762	-7.269	1.00 25.62 A
	ATOM	1067	CA	GLY A		69.963	14.972	-7.222	1.00 24.75 A
	MOTA	1068	C	GLY A		70.070	15.713	-5.908	1.00 25.82 A
	ATOM	1069	0	GLY A		69.080	16.241	-5.401	1.00 26.10 A
	MOTA	1070	N	ILE A	201	71.275	15.759	-5.353	1.00 25.31 A

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	ATOM	1071	CA	ILE A		71.490	16.440	-4.089	1.00 26.11 A
	MOTA	1072	CB	ILE A		71.886	15.438	-2.983	1.00 27.58 A
	MOTA	1073		ILE A		72.242	16.175	-1.704	1.00 27.99 A
	MOTA	1074	CG1	ILE A	201	70.725	14.480	-2.719	1.00 27.89 A
5	ATOM	1075	CD1	ILE A	201	71.068	13.366	-1.746	1.00 30.62 A
	MOTA	1076	C	ILE A	201	72.576	17.489	-4.233	1.00 25.92 A
	ATOM	1077	ō	ILE A		73.599	17.269	-4.887	1.00 25.94 A
	ATOM	1078	N	ILE A		72.337	18.640	-3.627	1.00 25.04 A
	ATOM	1079	CA	ILE A		73.289	19.733	-3.680	1.00 25.04 A
10									
10	MOTA	1080	CB	ILE A		72.640	20.990	-4.286	1.00 27.69 A
	MOTA	1081		ILE A		73.695	22.068	-4.516	1.00 30.47 A
	MOTA	1082		ILE A		71.992	20.639	-5.625	1.00 30.89 A
	MOTA	1083	CD1	ILE A	202	71.083	21.736	-6.178	1.00 31.79 A
	ATOM	1084	C	ILE A	202	73.742	20.032	-2.252	1.00 26.14 A
15	ATOM	1085	0	ILE A	202	72.912	20.201	-1.351	1.00 24.75 A
	MOTA	1086	N	HIS A	203	75.054	20.075	-2.042	1.00 25.17 A
	MOTA	1087	CA	HIS A		75.585	20.362	-0.717	1.00 24.36 A
	ATOM	1088	CB	HIS A		77.095	20.131	-0.677	1.00 23.06 A
	ATOM	1089	CG	HIS A		77.680	20.268	0.694	1.00 24.09 A
20	ATOM	1090		HIS A		77.956	21.366	1.434	1.00 24.05 A
20									
	ATOM	1091		HIS A		77.981	19.183	1.490	1.00 23.65 A
	MOTA	1092		HIS A		78.418	19.607	2.661	1.00 23.87 A
	MOTA	1093		HIS A		78.412	20.929	2.653	1.00 25.12 A
	MOTA	1094	С	HIS A		75.269	21.811	-0.330	1.00 24.71 A
25	ATOM	1095	0	HIS A	203	74.633	22.055	0.693	1.00 24.27 A
	ATOM	1096	N	ARG A	204	75.724	22.758	-1.154	1.00 25.89 A
	MOTA	1097	CA	ARG A	204	75.490	24.199	-0.961	1.00 25.68 A
	ATOM	1098	CB	ARG A		74.033	24.471	-0.596	1.00 25.57 A
	ATOM	1099	CG	ARG A		73.079	24.319	-1.751	1.00 29.26 A
30	ATOM	1100	CD	ARG A		71.815	25.118	-1.509	1.00 29.86 A
50	ATOM	1101	NE	ARG A		71.065	24.603	-0.373	1.00 23.00 A
	ATOM	1102	CZ	ARG A		70.021	25.219	0.170	1.00 36.01 A
	MOTA	1103		ARG A		69.607	26.383	-0.322	1.00 37.08 A
	MOTA	1104		ARG A		69.387	24.668	1.197	1.00 34.14 A
35	MOTA	1105	C	ARG A		76.373	24.935	0.034	1.00 26.91 A
	MOTA	1106	0	ARG A		76.210	26.144	0.243	1.00 26.29 A
	MOTA	1107	N	ASP A	205	77.303	24.221	0.654	1.00 26.23 A
	ATOM	1108	CA	ASP A	205	78.203	24.849	1.604	1.00 24.46 A
	ATOM	1109	CB	ASP A	205	77.557	24.909	2.990	1.00 28.25 A
40	ATOM	1110	CG	ASP A	205	78.203	25.954	3.890	1.00 30.95 A
	MOTA	1111	OD1	ASP A	205	78.872	26.862	3.354	1.00 35.13 A
	ATOM	1112		ASP A		78.034	25.880	5.127	1.00 33.48 A
	ATOM	1113	C	ASP A		79.483	24.039	1.631	1.00 24.22 A
	ATOM	1114	ō	ASP A		79.998	23.676	2.685	1.00 23.62 A
45	ATOM	1115	N	LEU A		79.995	23.755	0.442	1.00 23.31 A
43									
	MOTA	1116	CA	LEU A		81.206	22.978	0.321	1.00 24.19 A
	MOTA	1117	CB	LEU A		81.311	22.406	-1.088	1.00 24.78 A
	MOTA	1118	CG	LEU A		82.353	21.309	-1.285	1.00 25.24 A
	MOTA	1119		LEU A		82.075	20.173	-0.317	1.00 26.72 A
50	MOTA	1120	CD2	LEU A	206	82.298	20.808	-2.720	1.00 24.32 A
	ATOM	1121	C	LEU A	206	82.408	23.853	0.623	1.00 24.52 A
	ATOM	1122	0	LEU A	206	82.508	24.977	0.130	1.00 24.34 A
	ATOM	1123	N	LYS A	207	83.328	23.330	1.424	1.00 22.98 A
	ATOM	1124	CA	LYS A		84.517	24.083	1.796	1.00 23.05 A
55	ATOM	1125	CB	LYS A		84.113	25.305	2.629	1.00 21.18 A
55	ATOM	1126	CG	LYS A		83.278	24.948	3.830	1.00 21.10 A
	ATOM	1127	CD	LYS A		82.775	26.179	4.568	1.00 19.29 A 1.00 23.68 A
	MOTA	1128	CE	LYS A		81.913	25.781	5.767	1.00 21.99 A
	MOTA	1129	NZ	LYS A	207	81.580	26.910	6.686	1.00 25.14 A

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ATOM		ATOM	1130	C	LYS	Α	207	85.444	23.183	2.602	1.00 23.54 A
ATOM		ATOM	1131	0	LYS	Α	207	85.014	22.169	3.144	1.00 26.04 A
ATOM		MOTA	1132	N	PRO	Α	208	86.728	23.550	2.697	1.00 23.78 A
ATOM		MOTA	1133	CD	PRO	Α	208	87.309	24.764	2.100	1.00 21.90 A
ATOM	5	ATOM	1134	CA	PRO	А	208	87.754	22.801	3.429	1.00 23.64 A
ATOM		ATOM	1135	CB	PRO	А	208	88.948	23.750	3.397	1.00 22.67 A
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AROM 1157 CA ILEA 211 88.6733 18.174 4.043 1.00 21.36 A AROM 1159 CGB ILEA 211 86.676 18.538 2.744 1.00 20.33 6 A AROM 159 CGB ILEA 211 86.676 18.538 2.744 1.00 20.33 6 A AROM 160 CGI ILEA 211 88.475 19.089 1.719 1.00 20.04 A AROM 1160 CGI ILEA 211 88.475 19.089 1.719 1.00 20.56 A AROM 1162 CG ILEA 211 86.762 19.718 0.517 1.00 20.56 A AROM 1162 CG ILEA 211 86.733 17.629 5.048 1.00 22.45 A AROM 1163 OR ILEA 211 86.733 17.629 5.048 1.00 22.45 A AROM 1164 N LEU A 212 86.377 16.510 5.670 1.00 21.03 A AROM 1166 CB LEU A 212 86.377 16.510 5.670 1.00 21.03 A AROM 1166 CB LEU A 212 86.377 16.510 5.670 1.00 21.03 A AROM 1166 CB LEU A 212 86.370 16.520 5.685 1.00 20.43 A AROM 1166 CB LEU A 212 86.370 16.510 8.847 1.00 19.57 A AROM 1167 CG LEU A 212 86.370 17.592 8.817 1.00 19.57 A AROM 1169 CD2 LEU A 212 86.370 17.592 8.817 1.00 19.57 A AROM 1170 C LEU A 212 88.034 15.633 9.494 1.00 16.54 A AROM 1171 C LEU A 213 89.069 14.420 4.983 1.00 20.16 A AROM 1173 CA LEU A 213 89.069 14.420 4.983 1.00 20.16 A AROM 1173 CA LEU A 213 89.069 13.330 6.578 1.00 21.59 A AROM 1175 CG LEU A 213 89.991 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 89.991 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 89.991 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 89.991 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 89.991 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 89.991 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 89.912 12.151 7.554 1.00 22.98 A AROM 1177 CD LEU A 213 89.918 12.354 6.500 1.00 21.59 A AROM 1178 CD LEU A 213 89.918 12.354 6.700 1.00 22.95 A AROM 1178 CD LEU A 213 89.918 12.354 6.700 1.00 22.95 A AROM 1178 CD LEU A 213 89.918 12.354 6.700 22.95 A AROM 1180 CA ARN A 214 89.718 19.976 7.025 1.00 22.95 A AROM 1181 CA ARN A 214 89.718 19.976 7.705 0.50 23.75 AC1 AROM 1181 CA ARN A 214 89.718 19.976 7.705 0.50 23.75 AC1 AROM 1185 CO ARN A 214 89.718 12.934 8.268 1.00 23.66 A AROM 1185 CO ARN A 214 89.718 19.934 8.268 1.00 23.66 A AROM 1186 CO ARN A 214 89.718 19.934 8.268 1.00 23.66 A AROM 1186 CO ARN A 214 89.718 19.9				0							
AROM											
30 AROM 1159 CGZ ILE A 211 88.767 17.315 2.180 1.00 20.04 A AROM 1160 CGI ILE A 211 88.767 19.089 1.719 1.00 19.57 A AROM 1161 CDI ILE A 211 86.762 19.718 0.517 1.00 20.56 A AROM 1162 C ILE A 211 86.762 19.718 0.517 1.00 20.56 A AROM 1163 C ILE A 211 86.763 17.65 10.09 5.544 1.00 22.45 A AROM 1164 N LEU A 212 86.377 16.510 5.670 1.00 21.05 A AROM 1165 CA LEU A 212 86.377 16.510 5.670 1.00 21.05 A AROM 1166 CB LEU A 212 86.375 15.331 7.801 10.0 19.57 A AROM 1166 CB LEU A 212 86.352 15.331 7.801 10.0 19.57 A AROM 1168 CDI LEU A 212 86.352 15.331 7.801 10.0 19.57 A AROM 1168 CDI LEU A 212 86.352 15.331 7.801 10.0 19.57 A AROM 1169 CDI LEU A 212 88.540 15.631 9.494 1.00 19.58 A AROM 1170 C LEU A 212 88.540 15.633 15.613 9.494 1.00 16.55 A AROM 1171 O LEU A 212 88.034 14.420 4.983 1.00 20.95 A AROM 1171 O LEU A 212 88.034 14.420 4.983 1.00 20.95 A AROM 1173 CA LEU A 213 89.069 14.420 4.983 1.00 20.16 A AROM 1173 CA LEU A 213 89.069 13.330 6.578 1.00 21.16 A AROM 1176 CD LEU A 213 89.069 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 99.069 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 99.069 13.330 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 99.069 17.360 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 99.051 15.406 6.578 1.00 21.59 A AROM 1176 CD LEU A 213 99.051 15.406 6.578 1.00 21.59 A AROM 1177 CD LEU A 213 99.051 15.406 6.578 1.00 21.59 A AROM 1177 CD LEU A 213 99.051 15.406 6.578 1.00 21.59 A AROM 1177 CD LEU A 213 99.051 17.756 6.50 21.00 22.95 A AROM 1178 CD LEU A 213 99.912 12.161 7.554 1.00 22.95 A AROM 1180 CA ASN A 214 89.718 12.354 8.766 1.00 22.95 A AROM 1181 CA ASN A 214 89.718 12.354 8.766 1.00 22.59 A AROM 1181 CA ASN A 214 89.718 12.354 8.266 1.00 22.50 A AROM 1183 CO ASN A 214 89.718 12.354 8.263 0.50 25.62 AROM 1185 CO ASN A 214 89.718 12.354 8.268 1.00 23.66 A AROM 1185 CO ASN A 214 99.114 91.515 9.354 8.268 1.00 23.66 A AROM 1185 CO ASN A 214 99.115 9.354 8.288 1.00 23.66 A AROM 1186 CO ASN A 214 99.115 9.354 8.288 1.00 23.66 A AROM 1186 CO ASN A 214 99.115 9.354 8.288 1.00 23.66 A AROM 1186 CO A		MOTA	1157	CA	ILE	Α	211	85.733	18.174	4.043	1.00 21.36 A
AROM											
ATOM 1161 CD1 TLE A 211 86.733 17.629 5.048 1.00 22.45 A ATOM 1162 C TLE A 211 86.733 17.629 5.048 1.00 22.45 A ATOM 1163 O TLE A 211 86.733 17.629 5.048 1.00 22.45 A ATOM 1164 N LEU A 212 86.377 16.510 5.670 1.00 21.05 A ATOM 1165 CA LEU A 212 86.377 16.510 6.665 1.00 21.03 A ATOM 1166 CB LEU A 212 86.370 16.281 8.347 1.00 19.57 A ATOM 1166 CD1 LEU A 212 86.352 15.331 7.801 1.00 19.57 A ATOM 1168 CD1 LEU A 212 86.353 15.613 9.494 1.00 16.54 A ATOM 1169 CD2 LEU A 212 88.543 15.613 9.494 1.00 16.54 A ATOM 1170 C LEU A 212 88.034 17.592 8.817 1.00 19.57 A ATOM 1171 O LEU A 212 88.034 14.420 4.983 1.00 20.16 A ATOM 1173 C LEU A 213 89.069 14.379 6.578 1.00 21.07 A ATOM 1174 CB LEU A 213 89.069 14.379 6.578 1.00 21.07 A ATOM 1175 CC LEU A 213 89.069 14.379 6.578 1.00 21.07 A ATOM 1176 CD LEU A 213 89.069 14.379 6.578 1.00 21.07 A ATOM 1177 CD LEU A 213 89.069 14.379 6.578 1.00 21.58 A ATOM 1176 CD LEU A 213 91.633 14.944 5.400 1.00 21.25 A ATOM 1177 CD LEU A 213 91.633 14.944 5.400 1.00 21.25 A ATOM 1176 CD LEU A 213 91.633 14.944 5.400 1.00 21.25 A ATOM 1177 CD LEU A 213 91.633 14.944 5.400 1.00 21.25 A ATOM 1178 CD LEU A 213 91.633 14.944 5.400 1.00 21.25 A ATOM 1179 CD LEU A 213 91.633 14.944 5.400 1.00 21.25 A ATOM 1177 CD LEU A 213 91.633 14.944 5.400 1.00 21.25 A ATOM 1178 CD LEU A 213 91.578 14.335 4.070 1.00 22.35 A ATOM 1178 CD LEU A 213 89.912 12.151 7.554 1.00 22.28 A ATOM 1180 CD ASN A 214 89.718 9.765 7.767 1.00 22.95 A ATOM 1181 CD ASN A 214 89.718 9.765 7.755 0.50 23.75 AC1 ATOM 1183 CD ASN A 214 89.718 9.766 6.803 8.28 1.00 23.66 A ATOM 1185 ND ASN A 214 89.718 9.756 6.803 25.56 AC1 ATOM 1185 ND ASN A 214 89.718 9.756 6.803 8.28 1.00 23.66 A ATOM 1185 ND ASN A 214 89.718 9.756 6.803 25.64 AC1 ATOM 1185 ND ASN A 214 89.118 9.958 6.803 0.50 25.64 AC1 ATOM 1185 ND ASN A 214 99.115 9.354 8.288 1.00 23.66 A	30	ATOM	1159	CG2	ILE	Α	211	87.167	17.315	2.180	1.00 20.04 A
ATOM 1162 C ILE A 211 88.0733 17.629 5.048 1.00 22.45 A A A A A TOM 1163 C ILE A 211 87.805 18.209 5.254 1.00 21.87 A A TOM 1165 CA LEU A 212 86.377 16.510 5.670 1.00 21.03 A A TOM 1166 CB LEU A 212 86.375 16.201 5.670 1.00 21.03 A A TOM 1166 CB LEU A 212 86.352 15.331 7.801 1.00 19.57 A A TOM 1166 CB LEU A 212 86.352 15.331 7.801 1.00 19.57 A A TOM 1169 CD LEU A 212 88.245 15.613 7.801 1.00 19.57 A A TOM 1169 CD LEU A 212 88.5270 16.201 8.347 1.00 19.57 A A TOM 1170 C LEU A 212 88.148 14.833 6.139 1.00 20.45 A A TOM 1171 C LEU A 212 88.148 14.833 6.139 1.00 20.55 A A TOM 1172 N LEU A 213 88.034 14.420 4.983 1.00 20.16 A A TOM 1173 CA LEU A 213 88.093 17.300 6.578 1.00 21.07 A A TOM 1174 CB LEU A 213 89.991 13.330 6.578 1.00 21.07 A A TOM 1175 CG LEU A 213 99.915 13.300 6.578 1.00 21.07 A A TOM 1176 CD LEU A 213 99.915 13.404 5.440 1.00 21.02 6 A A TOM 1176 CD LEU A 213 99.915 15.460 6.520 1.00 21.07 A A TOM 1176 CD LEU A 213 99.915 15.466 5.501 1.00 21.07 A A TOM 1176 CD LEU A 213 99.915 15.460 6.520 1.00 21.07 A A TOM 1176 CD LEU A 213 99.915 15.460 6.520 1.00 21.07 A A TOM 1176 CD LEU A 213 99.15 15.460 6.520 1.00 21.07 A A TOM 1176 CD LEU A 213 99.15 15.460 6.520 1.00 21.07 A A TOM 1176 CD LEU A 213 99.15 15.460 6.520 1.00 21.07 A A TOM 1176 CD LEU A 213 99.15 15.460 6.520 1.00 22.96 A A TOM 1178 C LEU A 213 99.15 15.460 6.501 1.00 22.98 A A TOM 1178 C LEU A 213 99.15 15.460 1.00 22.28 A A TOM 1180 N ANN A 214 89.786 10.994 7.055 1.00 22.83 A A A TOM 1180 N ANN A 214 89.786 10.994 7.756 0.50 25.52 A C1 A TOM 1184 C A SNN A 214 89.786 10.994 7.756 0.50 25.52 A C1 A TOM 1185 N A SNN A 214 88.066 6.803 8.636 0.500 25.62 A AC1 A TOM 1185 N A SNN A 214 88.066 6.803 8.636 0.500 25.62 A AC1 A TOM 1185 N A SNN A 214 88.066 6.803 8.636 0.500 25.64 A AC1 A TOM 1185 N A SNN A 214 98.066 6.803 8.636 0.500 25.64 A AC1 A TOM 1185 N A SNN A 214 99.151 9.354 8.288 1.00 23.68 A A TOM 1186 C A SNN A 214 99.151 9.354 8.288 1.00 23.66 A A TOM 1186 C A SNN A 214 99.151 9.354 8.288 1.00 23.66 A A TOM 1186 C A SNN A 214 99.151 9.		ATOM	1160	CG1	ILE	Α	211	85.475	19.089	1.719	1.00 19.57 A
ATOM 1163 O TLE A 211 87.805 18.209 5.254 1.00 21.087 A 7 A 7 A 7 A 7 A 7 A 7 A 7 A 7 A 7 A		ATOM	1161	CD1	ILE	Α	211	86.162	19.718	0.517	1.00 20.56 A
35		MOTA	1162	С	ILE	Α	211	86.733	17.629	5.048	1.00 22.45 A
35		ATOM	1163	0	ILE	Α	211	87.805	18.209	5.254	1.00 21.87 A
ATOM 1165 CA LEU A 212 86.352 15.331 6.668 1.00 20.43 A ATOM 1166 CB LEU A 212 86.352 15.331 7.801 1.00 19.57 A ATOM 1167 CG LEU A 212 86.352 15.331 8.347 1.00 19.57 A 40 ATOM 1168 CD1 LEU A 212 86.352 15.331 9.494 1.00 19.57 A 40 ATOM 1170 C LEU A 212 88.148 15.613 9.494 1.00 19.58 A ATOM 1170 C LEU A 212 88.148 14.833 6.139 1.00 20.95 A ATOM 1171 C LEU A 212 88.148 14.833 1.00 20.16 A ATOM 1172 N LEU A 213 89.069 14.379 6.678 1.00 21.07 A ATOM 1173 CA LEU A 213 89.069 14.379 6.678 1.00 21.07 A ATOM 1173 CA LEU A 213 89.091 13.330 6.578 1.00 21.07 A ATOM 1175 CG LEU A 213 99.912 13.330 6.578 1.00 21.07 A ATOM 1176 CD LEU A 213 99.912 13.300 6.578 1.00 21.07 A ATOM 1176 CD LEU A 213 99.912 13.406 6.520 1.00 21.17 A ATOM 1176 CD LEU A 213 91.415 13.882 6.520 1.00 21.17 A ATOM 1177 CD LEU A 213 91.415 13.882 6.520 1.00 21.26 A ATOM 1178 CD LEU A 213 91.415 13.882 6.520 1.00 21.27 A ATOM 1177 CD LEU A 213 91.578 14.335 4.070 1.00 23.36 A ATOM 1178 CD LEU A 213 99.912 12.161 7.554 1.00 22.28 A ATOM 1180 CD LEU A 213 89.918 12.354 8.766 1.00 23.66 A ATOM 1180 CD ASN A 214 89.718 9.766 7.872 1.00 22.96 A ATOM 1181 CA ASN A 214 89.718 9.766 7.7872 1.00 22.95 A ATOM 1181 CA ASN A 214 89.718 9.766 7.7872 1.00 22.95 A ATOM 1183 CG ASN 214 89.718 9.766 7.756 0.50 25.52 AC1 ATOM 1185 ND ASN 214 89.914 7.286 7.756 0.50 25.52 AC1 ATOM 1185 ND ASN 214 89.914 9.151 9.354 8.288 1.00 23.66 A ATOM 1185 ND ASN 214 89.014 9.151 9.354 8.288 1.00 23.66 A ATOM 1185 ND ASN A 214 89.014 9.151 9.354 8.288 1.00 23.66 A ATOM 1185 ND ASN A 214 99.141 9.151 9.354 8.288 1.00 23.66 A ATOM 1185 ND ASN A 214 99.141 9.151 9.354 8.288 1.00 23.66 A ATOM 1187 O ASN A 214 99.141 9.151 9.354 8.288 1.00 23.66 A ATOM 1186 ND ASN A 214 99.141 9.151 9.354 8.288 1.00 23.66 A ATOM 1186 ND ASN A 214 99.141 9.151 9.354 8.288 1.00 23.66 A ATOM 1186 ND ASN A 214 99.141 9.151 9.354 8.288 1.00 23.66 A ATOM 1186 ND ASN A 214 99.151 9.354 8.288 1.00 23.66 A ATOM 1186 ND ASN A 214 99.151 9.354 8.288 1.00 23.66 A ATOM 1186 ND ASN A 214 99.151 9.354 8.288 1.00 23.66 A	35	ATOM		N	LEU	Α	212	86.377		5.670	1.00 21.03 A
ATOM		ATOM		CA	LEU	А	212	87.228	15.910	6.685	1.00 20.43 A
ATOM 1167 CG LEU A 212 88.5.270 16.281 8.347 1.00 19.01 A ATOM 1168 CD1 LEU A 212 88.5.343 15.613 9.494 1.00 16.54 A ATOM 1169 CD2 LEU A 212 88.5.03 17.592 8.817 1.00 19.58 A ATOM 1170 C LEU A 212 88.104 14.833 6.139 1.00 20.95 A ATOM 1171 O LEU A 212 88.104 14.823 4.893 1.00 20.16 A ATOM 1172 N LEU A 213 88.034 14.420 4.983 1.00 20.16 A ATOM 1173 CA LEU A 213 88.991 13.330 6.578 1.00 21.07 A ATOM 1174 CB LEU A 213 99.163 14.994 5.400 10.02 1.17 A ATOM 1175 CG LEU A 213 91.633 14.994 5.400 10.02 1.17 A ATOM 1176 CD1 LEU A 213 91.633 14.994 5.400 10.02 1.12 A ATOM 1177 CD2 LEU A 213 91.633 14.994 5.400 10.02 1.12 A ATOM 1177 CD2 LEU A 213 91.633 14.994 5.400 10.02 21.26 A ATOM 1178 CD LEU A 213 91.631 14.335 4.070 1.00 21.38 A ATOM 1179 CD2 LEU A 213 91.578 14.335 4.070 1.00 23.36 A ATOM 1180 C LEU A 213 89.912 12.354 8.766 1.00 22.58 A ATOM 1180 N ASN A 214 89.718 9.766 7.872 1.00 22.98 A ATOM 1181 CA ASN A 214 89.718 9.766 7.872 1.00 22.95 A ATOM 1181 CA ASN A 214 89.718 9.766 7.767 1.00 22.95 A ATOM 1183 CG ASN 214 89.718 9.766 7.755 0.50 25.52 AC1 ATOM 1184 CM ASN A 214 89.114 7.266 7.755 0.50 25.52 AC1 ATOM 1185 ND2 ASN 214 89.016 6.803 8.363 0.50 25.52 AC1 ATOM 1185 ND2 ASN 214 88.066 6.803 8.363 0.50 25.62 AC1 ATOM 1185 ND2 ASN 214 88.066 6.803 8.363 0.50 25.62 AC1 ATOM 1185 ND2 ASN 214 88.066 6.803 8.288 1.00 23.66 A ATOM 1185 ND2 ASN 214 88.066 6.803 8.288 1.00 23.66 A		ATOM	1166	CB	LEU	А	212	86.352	15.331	7.801	1.00 19.57 A
ATOM 1168 CD1 LEU A 212 85.903 17.502 8.817 1.00 16.54 A A TOM 1169 CD2 LEU A 212 85.903 17.502 8.817 1.00 19.58 A ATOM 1171 C LEU A 212 88.104 14.803 6.139 1.00 20.95 A ATOM 1171 C LEU A 212 88.034 14.400 4.983 1.00 20.95 A ATOM 1172 N LEU A 213 88.069 14.379 6.978 1.00 21.07 A ATOM 1173 CA LEU A 213 89.901 13.300 6.578 1.00 21.07 A ATOM 1174 CD LEU A 213 99.991 13.300 6.578 1.00 21.07 A ATOM 1175 CG LEU A 213 91.615 13.882 6.520 1.00 21.07 A ATOM 1176 CD LEU A 213 91.633 14.944 5.440 1.00 21.12 6 A ATOM 1176 CD LEU A 213 99.015 15.466 5.501 1.00 21.12 6 A ATOM 1177 CD2 LEU A 213 99.015 15.466 5.514 1.00 21.26 A ATOM 1179 CD LEU A 213 99.515 15.466 5.514 1.00 21.36 A ATOM 1179 CD LEU A 213 99.515 15.466 5.514 1.00 23.93 A ATOM 1178 C LEU A 213 89.912 12.161 7.554 1.00 22.28 A ATOM 1180 N ASN A 214 88.967 8.647 7.755 (1.00 22.83 A ATOM 1181 CA ASN A 214 88.9718 9.766 7.872 1.00 22.83 A ATOM 1182 CB ASN 214 88.9718 8.647 7.705 0.50 23.75 AC1 ATOM 1188 0 G ASN 214 88.914 7.266 7.756 0.50 23.75 AC1 ATOM 1185 NG ASN 214 88.916 6.803 8.363 0.50 25.62 AC1 ATOM 1185 NG ASN 214 88.066 6.803 8.363 0.50 25.64 AC1 ATOM 1185 NG ASN 214 88.066 6.803 8.363 0.50 25.64 AC1 ATOM 1186 C ASN A 214 88.066 6.803 8.363 0.50 25.64 AC1 ATOM 1186 C ASN A 214 88.066 6.803 8.363 0.50 25.64 AC1 ATOM 1186 C ASN A 214 88.066 6.803 8.363 0.50 25.64 AC1 ATOM 1186 C ASN A 214 98.1515 9.354 8.288 1.00 23.68 A		ATOM	1167	CG	LEU	А	212			8.347	1.00 19.01 A
40 ATOM 1169 CDZ LEU A 21Z 88.148 14.833 6.139 1.00 20.95 A ATOM 1170 C LEU A 21Z 88.148 14.833 6.139 1.00 20.95 A ATOM 1171 O LEU A 21Z 88.148 14.833 6.139 1.00 20.95 A ATOM 1172 N LEU A 21Z 88.034 14.420 4.983 1.00 20.16 A ATOM 1173 CA LEU A 21Z 88.034 14.420 4.983 1.00 20.16 A ATOM 1173 CA LEU A 21Z 88.991 13.330 6.578 1.00 21.07 A ATOM 1175 CG LEU A 21Z 91.632 15.382 6.520 1.00 21.07 A ATOM 1175 CG LEU A 21Z 91.632 15.486 5.501 4.00 21.26 A ATOM 1176 CD1 LEU A 21Z 93.051 15.466 5.514 1.00 21.26 A ATOM 1177 CDZ LEU A 21Z 91.632 14.335 4.070 1.00 23.36 A ATOM 1178 CDZ LEU A 21Z 91.632 15.466 5.514 1.00 23.28 A ATOM 1179 CDZ LEU A 21Z 91.632 15.466 5.514 0.00 21.26 A ATOM 1179 CDZ LEU A 21Z 91.578 14.335 4.070 1.00 23.36 A ATOM 1178 C LEU A 21Z 98.912 12.354 8.766 1.00 22.88 A ATOM 1180 N ASN A 214 98.912 12.354 8.766 1.00 22.89 A ATOM 1181 CA ASN A 214 98.786 10.99 7.025 1.00 22.95 A ATOM 1182 CB ASN 214 98.786 10.726 7.757 6.05 25.52 AC1 ATOM 1183 CG ASN 214 98.148 7.286 7.756 0.50 25.52 AC1 ATOM 1185 NDZ ASN 214 98.016 6.803 8.363 0.50 25.52 AC1 ATOM 1185 NDZ ASN 214 98.016 6.803 8.363 0.50 25.64 AC1 ATOM 1185 CD ASN A 214 98.016 6.803 8.363 0.50 25.64 AC1 ATOM 1186 C ASN A 214 98.1151 9.354 8.288 1.00 23.68 A ATOM 1186 C ASN A 214 98.1151 9.354 8.288 1.00 23.68 A											
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ATOM 1187 O ASN A 214 92.112 9.934 7.716 1.00 20.85 A											
ATOM 1188 N GLU A 215 91.291 8.379 9.119 1.00 25.06 A											
		MOTA	1188	N	GLU	Α	215	91.291	8.379	9.119	1.00 25.06 A

	MOTA	1189	CA	GLU	Α	215	92.603	7.901	9.545	1.00 26.20 A
	ATOM	1190	CB	GLU	Α	215	92.453	6.669	10.435	1.00 26.19 A
	ATOM	1191	CG	GLU	Α	215	93.770	6.153	10.985	1.00 29.08 A
	ATOM	1192	CD			215	93.589	4.963	11.907	0.00 28.21 A
5	ATOM	1193	OE1	GLU			93.064	3.927	11.449	0.00 28.42 A
	ATOM	1194		GLU			93.973	5.065	13.092	0.00 28.42 A
	ATOM	1195	C			215	93.532	7.566	8.385	1.00 26.12 A
	ATOM	1196	0	GLU			94.746	7.743	8.487	1.00 29.48 A
	ATOM	1197	N	ASP			92.976	7.070	7.287	1.00 25.52 A
10	MOTA	1198	CA	ASP	Α		93.798	6.728	6.133	1.00 25.79 A
	MOTA	1199	CB	ASP		216	93.164	5.564	5.376 0	.50 27.09 AC1
	MOTA	1200	CG	ASP		216	93.450	4.231	6.027 0	.50 29.11 AC1
	ATOM	1201	OD1	ASP		216	93.206	4.098	7.244 0	.50 31.09 AC1
	ATOM	1202	OD2	ASP		216	93.921	3.315	5.320 0	.50 31.52 AC1
15	ATOM	1203	С	ASP	А		94.034	7.896	5.173	1.00 24.88 A
	ATOM	1204	o	ASP			94.586	7.719	4.094	1.00 26.27 A
	ATOM	1205	N	MET			93.615	9.087	5.578	1.00 25.04 A
	ATOM	1206	CA	MET			93.789	10.301	4.792	1.00 24.86 A
			CB	MET		217	95.270			1.00 24.86 A
20	ATOM	1207						10.503	4.454	
20	MOTA	1208	CG	MET			96.139	10.834	5.676	1.00 29.66 A
	MOTA	1209	SD	MET			95.577	12.323	6.551	1.00 34.79 A
	MOTA	1210	CE	MET			96.130	13.598	5.411	1.00 30.61 A
	MOTA	1211	C	MET			92.942	10.437	3.528	1.00 24.93 A
	MOTA	1212	0	MET			93.277	11.215	2.629	1.00 23.08 A
25	ATOM	1213	N	HIS	Α	218	91.855	9.678	3.450	1.00 21.48 A
	MOTA	1214	CA	HIS	Α	218	90.947	9.799	2.319	1.00 21.72 A
	ATOM	1215	CB	HIS	Α	218	90.325	8.444	1.963	1.00 21.43 A
	ATOM	1216	CG	HIS	Α	218	91.225	7.578	1.138	1.00 24.55 A
	MOTA	1217		HIS			91.951	6.478	1.458	1.00 23.50 A
30	ATOM	1218		HIS			91.522	7.860	-0.179	1.00 23.64 A
	ATOM	1219		HIS			92.392	6.975	-0.633	1.00 21.12 A
	ATOM	1220		HIS			92.670	6.128	0.340	1.00 22.96 A
	ATOM	1221	C	HIS			89.891	10.785	2.812	1.00 20.49 A
			0						4.018	1.00 20.49 A
2.5	MOTA	1222		HIS			89.683	10.911		
35	ATOM	1223	N			219	89.231	11.488	1.897	1.00 18.82 A
	ATOM	1224	CA			219	88.244	12.473	2.306	1.00 17.27 A
	MOTA	1225	CB			219	87.914	13.487	1.178	1.00 15.59 A
	MOTA	1226		ILE			89.175	14.201	0.718	1.00 14.62 A
	MOTA	1227		ILE			87.252	12.769	0.006	1.00 16.04 A
40	MOTA	1228	CD1	ILE	Α	219	86.458	13.685	-0.888	1.00 15.29 A
	ATOM	1229	C	ILE	Α	219	86.934	11.885	2.772	1.00 17.64 A
	ATOM	1230	0	ILE	Α	219	86.564	10.774	2.402	1.00 18.93 A
	ATOM	1231	N	GLN	Α	220	86.240	12.658	3.597	1.00 19.19 A
	MOTA	1232	CA			220	84.933	12.293	4.119	1.00 21.50 A
45	MOTA	1233	CB			220	85.061	11.585	5.475	1.00 23.96 A
	ATOM	1234	CG			220	85.583	10.151	5.334	1.00 29.77 A
	ATOM	1235	CD			220	84.945	9.182	6.319	1.00 33.77 A
	ATOM	1236		GLN			85.257	9.188	7.513	1.00 37.87 A
50	MOTA	1237		GLN			84.040	8.347	5.821	1.00 34.29 A
50	MOTA	1238	C	GLN			84.158	13.599	4.240	1.00 21.53 A
	MOTA	1239	0			220	84.367	14.393	5.166	1.00 22.54 A
	MOTA	1240	N			221	83.284	13.833	3.270	1.00 19.63 A
	ATOM	1241	CA			221	82.498	15.054	3.234	1.00 19.30 A
	MOTA	1242	CB			221	82.055	15.366	1.785	1.00 20.41 A
55	MOTA	1243	CG2	ILE	Α	221	81.237	16.639	1.738	1.00 19.39 A
	MOTA	1244	CG1	ILE	Α	221	83.290	15.524	0.900	1.00 19.44 A
	ATOM	1245	CD1			221	82.977	15.802	-0.550	1.00 17.44 A
	ATOM	1246	C			221	81.284	14.951	4.141	1.00 18.36 A
	ATOM	1247	ō			221	80.627	13.911	4.204	1.00 15.98 A

	ATOM	1248	N	THR	Α	222	80.995	16.024	4.864	1.00	19.59 A	
	ATOM	1249	CA	THR	Α	222	79.844	16.008	5.753	1.00	22.76 A	
	MOTA	1250	CB	THR	Α	222	80.218	15.420	7.126	1.00	23.86 A	
	ATOM	1251	og1	THR			79.019	15.145	7.863		28.20 A	
5	ATOM	1252		THR			81.105	16.380	7.908	1.00		
-	ATOM	1253	C	THR			79.179	17.370	5.933	1.00		
	ATOM	1254	Ö	THR			79.505	18.334	5.229		25.65 A	
	ATOM	1255	N	ASP			78.248	17.427	6.881	1.00		
10	MOTA	1256	CA	ASP			77.449	18.611	7.202	1.00		
10	MOTA	1257	CB	ASP			78.303	19.865	7.422	1.00		
	MOTA	1258	CG	ASP			77.538	20.962	8.175	1.00		
	MOTA	1259		ASP			76.288	20.876	8.278		31.91 A	
	MOTA	1260	OD2	ASP	Α	223	78.177	21.911	8.671	1.00		
	ATOM	1261	C	ASP	Α	223	76.461	18.882	6.080	1.00	25.61 A	
15	MOTA	1262	0	ASP	Α	223	76.693	19.744	5.227	1.00	25.81 A	
	MOTA	1263	N	PHE	Α	224	75.358	18.139	6.098	1.00	25.18 A	
	MOTA	1264	CA	PHE	Α	224	74.310	18.266	5.096	1.00	26.75 A	
	ATOM	1265	CB	PHE			73.860	16.879	4.635		27.24 A	
	ATOM	1266	CG	PHE		224	74.857	16.189	3.753	1.00		
20	ATOM	1267	CD1	PHE			74.889	16.450	2.388	1.00		
	ATOM	1268	CD2	PHE		224	75.790	15.313	4.291	1.00		
	ATOM	1269	CE1	PHE			75.841	15.847	1.567	1.00		
	ATOM	1270	CE2	PHE			76.745	14.706	3.482	1.00		
		1271	CZ	PHE			76.770	14.708	2.117		30.54 A	
25	MOTA	1272						19.038	5.632		27.73 A	
23	MOTA		С	PHE			73.124					
	MOTA	1273	0	PHE			72.005	18.895	5.140		27.84 A	
	MOTA	1274	N	GLY			73.378	19.862	6.643		29.36 A	
	MOTA	1275	CA	GLY			72.319	20.656	7.235		30.10 A	
	MOTA	1276	С	GLY			71.825	21.741	6.297	1.00		
30	MOTA	1277	0			225	70.714	22.248	6.451	1.00		
	MOTA	1278	N	THR			72.640	22.091	5.311		29.95 A	
	ATOM	1279	CA	THR	Α	226	72.261	23.132	4.365	1.00	32.06 A	
	ATOM	1280	CB	THR	Α	226	73.381	24.167	4.226	1.00	33.35 A	
	ATOM	1281	OG1	THR	Α	226	74.454	23.608	3.455	1.00	35.74 A	
35	MOTA	1282	CG2	THR	Α	226	73.920	24.542	5.593	1.00	34.02 A	
	ATOM	1283	C	THR	Α	226	71.979	22.551	2.983	1.00	31.11 A	
	ATOM	1284	0	THR	А	226	71.801	23.288	2.012	1.00	30.89 A	
	ATOM	1285	N	ALA	А	227	71.938	21.230	2.899	1.00	30.02 A	
	ATOM	1286	CA	ALA			71.714	20.566	1.624		32.20 A	
40	ATOM	1287	CB	ALA			71.906	19.057	1.770	1.00		
	ATOM	1288	c	ALA			70.345	20.865	1.045	1.00		
	ATOM	1289	ŏ	ALA			69.431	21.269	1.761	1.00		
	ATOM	1290	N	ALA			70.229	20.684	-0.266	1.00		
	ATOM	1291	CA	ALA			68.980	20.902	-0.982		34.43 A	
45			CB	ALA				22.146			32.03 A	
43	ATOM	1292					69.079		-1.861			
	MOTA	1293	C	ALA			68.742	19.674	-1.846		35.25 A	
	MOTA	1294	0	ALA			69.612	19.284	-2.622		36.70 A	
	MOTA	1295	N	VAL			67.578	19.056	-1.698		36.21 A	
	MOTA	1296	CA	VAL			67.246	17.876	-2.488		37.95 A	
50	MOTA	1297	CB	VAL			66.438	16.857	-1.674	1.00		
	MOTA	1298		VAL			66.192	15.609	-2.506	1.00		
	MOTA	1299		VAL			67.176	16.522	-0.394	1.00		
	MOTA	1300	C	VAL	Α	229	66.393	18.341	-3.649	1.00	40.15 A	
	ATOM	1301	0	VAL	Α	229	65.353	18.965	-3.446	1.00	39.20 A	
55	ATOM	1302	N	LEU	Α	230	66.836	18.044	-4.865	1.00	43.75 A	
	MOTA	1303	CA	LEU			66.105	18.455	-6.054	1.00		
	ATOM	1304	CB	LEU		230	67.039	18.473	-7.258	1.00		
	ATOM	1305	CG	LEU			68.123	19.552	-7.212		50.35 A	
	ATOM	1306	CD1	LEU			69.118	19.312	-8.326		50.62 A	

	ATOM	1307	CD2	LEU	-	220	67.488	20.932	-7.330	1 00	50.11	76
	MOTA	1308	C	LEU			64.905	17.569	-6.346		51.38	
	MOTA	1309	0	LEU			64.929	16.364	-6.095		51.84	
	MOTA	1310	N	SER	Α	231	63.854	18.190	-6.872	1.00	56.03	A
5	MOTA	1311	CA	SER	Α	231	62.616	17.502	-7.224	1.00	60.24	Α
	MOTA	1312	CB	SER	Α	231	61.528	17.806	-6.186	1.00	60.77	A
	ATOM	1313	OG	SER	А	231	61.222	19.192	-6.150	1.00	61.08	A
	ATOM	1314	C	SER			62.115	17.894	-8.622			Α
	ATOM	1315	0	SER			61.527	17.068	-9.326		63.42	A
10	ATOM	1316	N	PRO			62.334	19.161	-9.040		64.66	
10	ATOM	1317	CD	PRO			62.903	20.298	-8.289		64.95	
	MOTA	1318	CA	PRO			61.882		-10.367			A
	MOTA	1319	CB	PRO			62.409	21.037	-10.450			A
	MOTA	1320	CG	PRO			62.341	21.493	-9.031			A
15	MOTA	1321	C	PRO			62.408		-11.505			A
	MOTA	1322	0	PRO	Α	232	62.858	19.241	-12.532	1.00	66.55	A
	MOTA	1323	N	ALA	Α	239	65.927	26.021	-3.995	1.00	92.57	Α
	ATOM	1324	CA	ALA	Α	239	67.330	26.100	-3.606	1.00	92.64	А
	ATOM	1325	CB	ALA	А	239	68.187	25.262	-4.558	1.00	92.15	A
20	ATOM	1326	c	ALA			67.769	27.558	-3.640			A
20	ATOM	1327	ŏ	ALA			68.683	27.930	-4.373		92.47	
		1328	N	ASN			67.108	28.379	-2.833		91.92	
	MOTA											
	MOTA	1329	CA	ASN			67.396	29.809	-2.767		91.12	
	MOTA	1330	CB	ASN			66.374	30.566	-3.617			A
25	MOTA	1331	CG	ASN			64.947	30.084	-3.378		93.20	
	MOTA	1332		ASN			64.471	30.061	-2.244		93.46	
	MOTA	1333	ND2	ASN	Α	240	64.261	29.697	-4.452	1.00	94.00	A
	MOTA	1334	C	ASN	Α	240	67.334	30.332	-1.335	1.00	89.78	A
	MOTA	1335	0	ASN	Α	240	67.766	31.453	-1.053	1.00	89.80	Α
30	MOTA	1336	N	ALA	Α	241	66.787	29.515	-0.441	1.00	88.16	A
	MOTA	1337	CA	ALA	А	241	66.624	29.891	0.955	1.00	86.55	А
	ATOM	1338	С	ALA			67.901	29.893	1.792		84.55	
	ATOM	1339	ō	ALA			67.865	30.268	2.961		84.76	
	ATOM	1340	CB	ALA			65.583	28.978	1.623		88.01	
35	ATOM	1341	N	PHE			69.028	29.494	1.216		82.28	
33		1342						29.494				
	MOTA		CA	PHE			70.264		1.993		79.83	
	MOTA	1343	CB	PHE			70.718	28.046	2.282		79.60	
	MOTA	1344	CG	PHE			71.980	27.962	3.100		79.10	
	MOTA	1345		PHE			72.024	28.483	4.388		79.45	
40	MOTA	1346		PHE			73.131	27.392	2.571		79.42	
	MOTA	1347		PHE			73.202	28.442	5.143		79.29	
	MOTA	1348	CE2	PHE	Α	242	74.314	27.345	3.317	1.00	80.20	A
	MOTA	1349	CZ	PHE	Α	242	74.348	27.872	4.605	1.00	79.98	A
	MOTA	1350	C	PHE	Α	242	71.402	30.231	1.322	1.00	77.56	A
45	MOTA	1351	0	PHE	Α	242	71.347	30.524	0.130	1.00	78.59	Α
	MOTA	1352	N	VAL			72.440	30.529	2.098		73.76	
	ATOM	1353	CA	VAL			73.595	31.238	1.579		70.34	
	ATOM	1354	CB	VAL			73.864	32.515	2.405		71,71	
	ATOM	1355		VAL			75.087	33.238	1.859		71.29	
50	ATOM	1356		VAL			72.638	33.425	2.376		71.41	
50												
	MOTA	1357	С	VAL			74.851	30.362	1.581		66.69	
	MOTA	1358	0	VAL			75.232	29.802	0.552		66.50	
	MOTA	1359	N	GLY			75.496	30.245	2.737		62.34	
	MOTA	1360	CA	GLY			76.708	29.444	2.829		56.48	Α
55	MOTA	1361	C	GLY			77.889	30.327	3.168			Α
	MOTA	1362	0	GLY	Α	244	77.769	31.547	3.136	1.00	52.14	Α
	MOTA	1363	N	THR	Α	245	79.031	29.733	3.490	1.00	48.25	Α
	MOTA	1364	CA	THR			80.201	30.530	3.838		44.49	
	ATOM	1365	CB	THR			81.413	29.633	4.106		45.53	
	111 011	1505		1.111			01.115	25.055	1.100	1.00	10.00	

	ATOM	1366	OG1	THR	Α	245	80.994	28.514	4.899	1.00 45.14 A
	ATOM	1367	CG2	THR	Α	245	82.486	30.403	4.873	1.00 42.13 A
	MOTA	1368	C	THR	Α	245	80.523	31.537	2.734	1.00 40.69 A
	ATOM	1369	0	THR	Α	245	80.722	31.175	1.572	1.00 38.45 A
5	ATOM	1370	N	ALA	Α	246	80.570	32.804	3.127	1.00 36.53 A
	MOTA	1371	CA	ALA	А	246	80.816	33.915	2.219	1.00 34.68 A
	ATOM	1372	CB	ALA			81,106	35.186	3.023	1.00 34.13 A
	ATOM	1373	c	ALA			81.896	33.718	1.164	1.00 33.21 A
	ATOM	1374	ō	ALA			81.655	33.958	-0.015	1.00 33.62 A
10	ATOM	1375	N	GLN		247	83.082	33.281	1.567	1.00 31.02 A
	ATOM	1376	CA	GLN			84.151	33.112	0.595	1.00 31.05 A
	ATOM	1377	CB	GLN		247	85.476	32.814	1.310	1.00 33.25 A
	ATOM	1378	CG	GLN			85.921	33.931	2.253	1.00 37.08 A
	ATOM	1379	CD	GLN		247	87.378	33.831	2.665	1.00 40.56 A
15	ATOM	1380		GLN			88.272	34.328	1.972	1.00 40.30 A
15	ATOM	1381	NE2	GLN			87.626	33.180	3.794	1.00 41.24 A
	ATOM	1382	C	GLN			83.895	32.069	-0.488	1.00 28.53 A
	ATOM	1383	0	GLN			84.544	32.093	-1.527	1.00 27.93 A
				TYR			82.934			
20	ATOM	1384	N	TYR			82.643	31.177	-0.267 -1.238	1.00 28.01 A 1.00 28.20 A
20	ATOM	1385	CA	TYR			82.725	28.757	-0.532	
	ATOM	1386	CB							
	ATOM	1387	CG	TYR		248	84.064	28.533	0.126	1.00 23.77 A
	MOTA	1388		TYR			85.153	28.073	-0.611	1.00 23.01 A
2.5	MOTA	1389	CE1	TYR			86.421	27.975	-0.039	1.00 24.66 A
25	MOTA	1390	CD2	TYR			84.270	28.879	1.464	1.00 24.01 A
	MOTA	1391	CE2	TYR			85.535	28.785	2.050	1.00 24.49 A
	MOTA	1392	CZ	TYR			86.606	28.338	1.286	1.00 26.11 A
	MOTA	1393	OH	TYR			87.868	28.305	1.828	1.00 27.54 A
	MOTA	1394	C	TYR			81.301	30.249	-1.961	1.00 28.78 A
30	MOTA	1395	0	TYR		248	80.939	29.405	-2.777	1.00 30.26 A
	MOTA	1396	N	VAL			80.576	31.319	-1.663	1.00 28.83 A
	ATOM	1397	CA	VAL			79.281	31.584	-2.275	1.00 28.70 A
	MOTA	1398	CB	VAL			78.625	32.803	-1.601	1.00 29.37 A
	MOTA	1399		VAL		249	77.333	33.163	-2.297	1.00 30.56 A
35	ATOM	1400		VAL			78.376	32.488	-0.127	1.00 31.25 A
	ATOM	1401	C	VAL			79.404	31.837	-3.779	1.00 28.19 A
	MOTA	1402	0	VAL			80.335	32.497	-4.231	1.00 27.69 A
	MOTA	1403	N	SER			78.460	31.308	-4.549	1.00 28.16 A
	MOTA	1404	CA	SER			78.476	31.481	-5.993	1.00 29.05 A
40	MOTA	1405	CB	SER			77.835	30.273	-6.691	1.00 31.08 A
	MOTA	1406	OG	SER	Α	250	76.497	30.058	-6.264	1.00 31.33 A
	MOTA	1407	C	SER	Α	250	77.737	32.752	-6.376	1.00 29.69 A
	MOTA	1408	0	SER	Α	250	76.820	33.191	-5.685	1.00 29.14 A
	MOTA	1409	N	PRO	Α	251	78.131	33.361	-7.494	1.00 29.35 A
45	MOTA	1410	CD	PRO	Α	251	79.147	32.917	-8.463	1.00 29.28 A
	MOTA	1411	CA	PRO	Α	251	77.477	34.592	-7.934	1.00 30.27 A
	MOTA	1412	CB	PRO	Α	251	78.214	34.932	-9.235	1.00 29.87 A
	ATOM	1413	CG	PRO	Α	251	78.687	33.588	-9.730	1.00 30.48 A
	ATOM	1414	C	PRO	Α	251	75.961	34.495	-8.114	1.00 30.86 A
50	ATOM	1415	0	PRO	Α	251	75.246	35.442	-7.801	1.00 33.28 A
	ATOM	1416	N	GLU	А	252	75.459	33.367	-8.602	1.00 30.19 A
	ATOM	1417	CA	GLU			74.014	33.244	-8.802	1.00 30.91 A
	ATOM	1418	CB	GLU			73.649	31.903	-9.449	1.00 30.61 A
	ATOM	1419	CG	GLU		252	74.162	30.682	-8.689	1.00 33.88 A
55	ATOM	1420	CD	GLU			75.493	30.171	-9.219	1.00 32.82 A
	ATOM	1421	OE1	GLU			76.277	30.987	-9.747	1.00 35.25 A
	ATOM	1422		GLU			75.756	28.956	-9.095	1.00 33.23 A
	ATOM	1423	C	GLU			73.260	33.390	-7.494	1.00 32.11 A
	ATOM	1424	0	GLU			72.157	33.928	-7.469	1.00 32.03 A
	ALOH	1124	0	SHO	Λ			55.520	7.403	1.00 J2.01 A

	ATOM	1425	N	LEU	А	253	73.852	32.900	-6.408	1.00	33.87	А
	ATOM	1426	CA	LEU			73.230	32.988	-5.096			A
	ATOM	1427	CB	LEU			74.031	32.183	-4.078			A
	ATOM	1428	CG	LEU			73.371	30.937	-3.479		40.98	A
5												
3	ATOM	1429		LEU		253	74.302	30.321	-2.433		42.16	Α
	MOTA	1430		LEU			72.043	31.314	-2.835			Α
	ATOM	1431	C	LEU			73.148	34.445	-4.640			Α
	ATOM	1432	0	LEU			72.300	34.810	-3.820			А
	ATOM	1433	N	LEU			74.036	35.276	-5.171			А
10	ATOM	1434	CA	LEU			74.052	36.686	-4.816			Α
	MOTA	1435	CB	LEU	Α	254	75.481	37.235	-4.890	1.00	35.47	Α
	ATOM	1436	CG	LEU	Α	254	76.512	36.692	-3.899	1.00	32.31	Α
	ATOM	1437	CD1	LEU	Α	254	77.839	37.416	-4.108	1.00	32.18	Α
	ATOM	1438	CD2	LEU	Α	254	76.019	36.891	-2.474			Α
15	ATOM	1439	C	LEU	Α	254	73.150	37.496	-5.737	1.00	39.82	Α
	ATOM	1440	o	LEU			72.772	38.615	-5.409			А
	ATOM	1441	N	THR			72.805	36.919	-6.885		44.09	
	ATOM	1442	CA	THR			71.959	37.594	-7.865		47.95	
	ATOM	1443	CB	THR			72.591	37.544	-9.276			A
20	ATOM	1444		THR			73.924	38.072	-9.227			A
20	ATOM	1445	CG2	THR			71.768		-10.253			A
	ATOM	1446	C	THR			70.538	37.032	-7.954			A
	MOTA	1447	0	THR			69.631	37.537	-7.300			A
2.5	ATOM	1448	N	GLU			70.344	35.994	-8.764		52.84	A
25	ATOM	1449	CA	GLU			69.018	35.395	-8.939		55.77	А
	ATOM	1450	CB	GLU			69.036		-10.061		55.24	А
	MOTA	1451	CG	GLU			70.360		-10.790			Α
	MOTA	1452	CD	GLU		256	70.699		-11.681		55.34	А
	MOTA	1453	OE1	GLU	Α	256	69.831		-12.480			А
30	ATOM	1454	OE2	GLU	Α	256	71.837	35.852	-11.593	0.00	55.36	Α
	MOTA	1455	C	GLU	Α	256	68.451	34.743	-7.677	1.00	57.04	Α
	ATOM	1456	0	GLU	Α	256	67.396	34.107	-7.732	1.00	56.82	Α
	ATOM	1457	N	LYS	Α	257	69.137	34.911	-6.549	1.00	58.87	Α
	ATOM	1458	CA	LYS	Α	257	68.711	34.308	-5.286	1.00	60.38	Α
35	ATOM	1459	CB	LYS	Α	257	67.607	35.151	-4.623	1.00	60.84	Α
	ATOM	1460	CG	LYS			66.327	35.322	-5.430		60.71	
	ATOM	1461	CD	LYS			65.352	36.261	-4.731			A
	ATOM	1462	CE	LYS			64.943	35.734	-3.363		60.77	
	ATOM	1463	NZ	LYS			63.992	36.650	-2.674			A
40	ATOM	1464	C	LYS			68.227	32.878	-5.546			A
40	ATOM	1465	ō	LYS			67.046	32.565	-5.389		61.84	
	ATOM	1466	N	SER			69.160	32.020	-5.958		61.26	
	ATOM	1467	CA	SER			68.865	30.622	-6.271		61.31	
	ATOM	1468	CB	SER			68.105	30.548	-7.605		62.95	
45												
45	MOTA	1469	OG	SER			68.707	31.374	-8.596		63.22	
	MOTA	1470	С	SER			70.149	29.771	-6.334		60.39	
	MOTA	1471	0	SER			71.257	30.312	-6.329			А
	MOTA	1472	N	ALA			70.001	28.447	-6.393			А
	MOTA	1473	CA	ALA			71.159	27.551	-6.441			А
50	MOTA	1474	CB	ALA			71.670	27.289	-5.025		54.90	
	ATOM	1475	C	ALA			70.890	26.218	-7.147		52.13	Α
	ATOM	1476	0	ALA	Α	259	69.759	25.726	-7.175	1.00	51.63	Α
	ATOM	1477	N	CYS	Α	260	71.945	25.641	-7.712	1.00	48.49	Α
	MOTA	1478	CA	CYS	Α	260	71.848	24.371	-8.417	1.00	44.82	Α
55	ATOM	1479	CB	CYS	Α	260	71.499	24.596	-9.890	1.00	46.78	Α
	ATOM	1480	SG	CYS		260	72.731	25.549	-10.821			А
	ATOM	1481	C	CYS		260	73.176	23.643	-8.310			Α
	ATOM	1482	Ö	CYS			74.085	24.090	-7.612		41.05	
	ATOM	1483	N	LYS			73.288	22.525	-9.012		37.76	
									011			

	ATOM	1484	0.7	LYS	2	261	74.503	21.729	-8.980	1.00 3	4 00 *	
			CA	LYS			74.303		-8.980	1.00 3		
	MOTA	1485	CB					20.587				
	MOTA	1486	CG	LYS			73.239	19.644	-9.691	1.00 3		
	MOTA	1487	CD	LYS			73.239		-10.601	1.00 3		
5	ATOM	1488	CE	LYS			72.117		-10.229	1.00 4		
	MOTA	1489	NZ	LYS .	Α	261	72.076	16.269	-11.110	1.00 4	1.64 A	
	ATOM	1490	C	LYS	Α	261	75.751	22.556	-9.247	1.00 3	2.19 A	
	MOTA	1491	0	LYS	Α	261	76.780	22.366	-8.595	1.00 3	0.08 A	
	ATOM	1492	N	SER	Α	262	75.651	23.480	-10.200	1.00 3	0.41 A	
10	ATOM	1493	CA	SER	Α	262	76.771	24.337	-10.556	1.00 2	7.88 A	
	ATOM	1494	CB	SER	А	262	76.361	25.333	-11.643	1.00 2	9.04 A	
	ATOM	1495	OG	SER			76.398		-12.921	1.00 3		
	ATOM	1496	C	SER			77.325	25.095	-9.360	1.00 2		
	ATOM	1497	ō	SER			78.515	25.403	-9.320	1.00 2		
15	ATOM	1498	N	SER			76.469	25.406	-8.392	1.00 2		
15	ATOM	1499	CA	SER			76.924	26.115	-7.201	1.00 2		
				SER			75.758		-6.242			
	ATOM	1500	CB					26.354		1.00 2		
	ATOM	1501	OG	SER			74.830	27.254	-6.832	1.00 3		
	MOTA	1502	C	SER			78.039	25.337	-6.506	1.00 2		
20	MOTA	1503	0	SER			79.034	25.924	-6.078	1.00 2		
	MOTA	1504	N	ASP.			77.884	24.019	-6.396	1.00 2		
	MOTA	1505	CA	ASP.			78.930	23.215	-5.773	1.00 2		
	ATOM	1506	CB	ASP.	Α	264	78.500	21.754	-5.613	1.00 2	3.87 A	
	ATOM	1507	CG	ASP.	Α	264	77.378	21.577	-4.599	1.00 2	7.11 A	
25	ATOM	1508	OD1	ASP.	Α	264	77.276	22.402	-3.662	1.00 2	5.60 A	
	ATOM	1509	OD2	ASP.	Α	264	76.612	20.599	-4.730	1.00 2	6.16 A	
	ATOM	1510	С	ASP.	А	264	80.175	23.267	-6.642	1.00 2	0.62 A	
	ATOM	1511	0	ASP.			81.289	23.339	-6.129	1.00 2		
	ATOM	1512	N	LEU			79.985	23.246	-7.959	1.00 1		
30	ATOM	1513	CA	LEU			81.113	23.275	-8.876	1.00 2		
30	ATOM	1514	CB	LEU			80.634		-10.322	1.00 1		
	ATOM	1515	CG	LEU			80.037		-10.672	1.00 2		
	ATOM	1516		LEU			79.580		-12.122	1.00 2		
	ATOM	1517		LEU			81.077		-10.449	1.00 2		
25												
35	ATOM	1518	C	LEU .			81.910	24.552	-8.705	1.00 2		
	ATOM	1519	0	LEU .			83.130	24.563	-8.881	1.00 2		
	MOTA	1520	N	TRP			81.221	25.633	-8.361	1.00 2		
	MOTA	1521	CA	TRP			81.897	26.899	-8.138	1.00 2		
40	MOTA	1522	CB	TRP			80.879	28.031	-7.960	1.00 2		
40	MOTA	1523	CG	TRP			81.477	29.309	-7.411	1.00 2		
	MOTA	1524		TRP			81.814	30.487	-8.152	1.00 2		
	MOTA	1525		TRP			82.391	31.404	-7.243	1.00 2		
	ATOM	1526		TRP			81.689	30.858	-9.497	1.00 2	4.79 A	
	MOTA	1527		TRP			81.850	29.555	-6.116	1.00 2		
45	ATOM	1528	NE1	TRP	Α	266	82.401	30.811	-6.009	1.00 2	3.65 A	
	ATOM	1529	CZ2	TRP	Α	266	82.839	32.663	-7.636	1.00 2	2.89 A	
	ATOM	1530	CZ3	TRP	Α	266	82.139	32.116	-9.887	1.00 2	3.30 A	
	ATOM	1531	CH2	TRP	A	266	82.705	33.000	-8.959	1.00 2	3.32 A	
	ATOM	1532	C	TRP	Α	266	82.739	26.735	-6.877	1.00 2	0.30 A	
50	ATOM	1533	0	TRP			83.913	27.102	-6.853	1.00 2		
	ATOM	1534	N	ALA			82.141	26.175	-5.832	1.00 1		
	ATOM	1535	CA	ALA			82.868	25.966	-4.584	1.00 1		
	ATOM	1536	CB	ALA			81.984	25.254	-3.561	1.00 1		
	ATOM	1537	C	ALA			84.112	25.132	-4.877	1.00 1		
55		1537	0	ALA				25.132	-4.877	1.00 1		
33	ATOM						85.173					
	ATOM	1539	N	LEU			83.982	24.190	-5.799	1.00 1		
	ATOM	1540	CA	LEU .			85.118	23.355	-6.157	1.00 1		
	MOTA	1541	CB	LEU			84.703	22.326	-7.204	1.00 1		
	MOTA	1542	CG	LEU	A	268	85.809	21.436	-7.772	1.00 1	6.93 A	

	ATOM	1543		LEU			86.333	20.495	-6.704	1.00 17.10 A
	ATOM	1544	CD2	LEU	Α	268	85.258	20.651	-8.953	1.00 13.46 A
	ATOM	1545	C	LEU	Α	268	86.232	24.249	-6.705	1.00 19.64 A
	ATOM	1546	0	LEU	А	268	87.389	24.129	-6.306	1.00 18.99 A
5	ATOM	1547	N	GLY			85.869	25.158	-7.606	1.00 19.16 A
	ATOM	1548	CA	GLY			86.854	26.057	-8.178	1.00 18.25 A
	ATOM	1549	C	GLY			87.604	26.804	-7.103	1.00 20.30 A
	MOTA	1550	0	GLY			88.825	26.960	-7.178	1.00 20.24 A
	MOTA	1551	N	CYS			86.874	27.266	-6.090	1.00 20.20 A
10	MOTA	1552	CA	CYS	Α	270	87.486	27.996	-4.986	1.00 20.73 A
	MOTA	1553	CB	CYS	Α	270	86.418	28.523	-4.031	1.00 21.05 A
	ATOM	1554	SG	CYS	Α	270	85.292	29.703	-4.752	1.00 23.98 A
	ATOM	1555	C	CYS	А	270	88.417	27.082	-4.206	1.00 20.77 A
	ATOM	1556	0	CYS			89.550	27.449	-3.878	1.00 22.00 A
15	ATOM	1557	N	ILE			87.927	25.886	-3.907	1.00 19.32 A
	ATOM	1558	CA	ILE			88.704	24.921	-3.147	1.00 18.46 A
	ATOM	1559	CB	ILE			87.872	23.668	-2.861	1.00 15.71 A
	MOTA	1560		ILE			88.722	22.607	-2.182	1.00 16.51 A
	MOTA	1561		ILE			86.688	24.051	-1.974	1.00 14.97 A
20	ATOM	1562	CD1	ILE			85.785	22.891	-1.639	1.00 17.80 A
	MOTA	1563	C	ILE	Α	271	90.001	24.546	-3.856	1.00 19.30 A
	ATOM	1564	0	ILE	Α	271	91.062	24.532	-3.242	1.00 21.30 A
	ATOM	1565	N	ILE	Α	272	89.915	24.253	-5.147	1.00 20.07 A
	ATOM	1566	CA	ILE	А	272	91.094	23.894	-5.906	1.00 21.50 A
25	ATOM	1567	CB	ILE			90.758	23.693	-7.385	1.00 22.57 A
	ATOM	1568	CG2	ILE			92.041	23.498	-8.184	1.00 21.91 A
	ATOM	1569		ILE			89.818	22.495	-7.542	1.00 23.57 A
	ATOM	1570		ILE			89.314	22.294	-8.949	1.00 23.37 A
			CDI							
20	MOTA	1571		ILE			92.112	25.010	-5.794	1.00 22.90 A
30	MOTA	1572	0	ILE			93.287	24.783	-5.507	1.00 21.82 A
	MOTA	1573	N	TYR			91.638	26.226	-6.028	1.00 24.81 A
	MOTA	1574	CA	TYR			92.478	27.400	-5.969	1.00 25.15 A
	MOTA	1575	CB	TYR			91.630	28.632	-6.255	1.00 26.04 A
	ATOM	1576	CG	TYR	Α	273	92.385	29.931	-6.173	1.00 27.80 A
35	ATOM	1577	CD1	TYR	Α	273	92.715	30.500	-4.939	1.00 27.53 A
	ATOM	1578	CE1	TYR	А	273	93.405	31.708	-4.870	1.00 27.30 A
	ATOM	1579	CD2	TYR			92.765	30.602	-7.333	1.00 27.17 A
	ATOM	1580	CE2	TYR			93.448	31.804	-7.277	1.00 26.68 A
	ATOM	1581	CZ	TYR			93.766	32.355	-6.050	1.00 28.05 A
40	ATOM	1582	OH	TYR			94.433	33.562	-6.018	1.00 30.80 A
40	ATOM	1583	C	TYR			93.139	27.521	-4.599	1.00 26.05 A
	ATOM	1584	0	TYR			94.310	27.889	-4.489	1.00 24.45 A
	ATOM	1585	N	GLN			92.380	27.205	-3.556	1.00 25.95 A
	ATOM	1586	CA	GLN			92.896	27.299	-2.202	1.00 25.98 A
45	ATOM	1587	CB	GLN			91.743	27.209	-1.199	1.00 25.56 A
	MOTA	1588	CG	GLN			92.169	27.422	0.233	1.00 25.42 A
	MOTA	1589	CD	GLN			90.990	27.571	1.161	1.00 28.69 A
	ATOM	1590	OE1	GLN	Α	274	89.838	27.506	0.732	1.00 29.84 A
	ATOM	1591	NE2	GLN	Α	274	91.267	27.774	2.445	1.00 29.83 A
50	MOTA	1592	C	GLN	Α	274	93.951	26.231	-1.915	1.00 25.08 A
	MOTA	1593	0	GLN			94.862	26.452	-1.120	1.00 24.38 A
	ATOM	1594	N	LEU			93.838	25.081	-2.567	1.00 24.42 A
	ATOM	1595	CA	LEU			94.813	24.006	-2.369	1.00 25.43 A
	ATOM	1595	CB	LEU			94.813	22.713	-3.035	1.00 25.43 A
55	MOTA	1597	CG	LEU			93.193	21.959	-2.354	1.00 25.67 A
	MOTA	1598		LEU			92.817	20.702	-3.154	1.00 22.16 A
	MOTA	1599		LEU			93.633	21.580	-0.950	1.00 23.32 A
	MOTA	1600	C	LEU			96.171	24.376	-2.948	1.00 25.40 A
	MOTA	1601	0	LEU	Α	275	97.212	24.071	-2.376	1.00 25.87 A

	ATOM	1602	N	VAL	2	276	96.153	25.039	-4.094	1 00	25.78 A
	MOTA	1603	CA	VAL			97.384	25.419	-4.759		26.12 A
	MOTA	1604	CB	VAL			97.170	25.522	-6.280		26.14 A
	MOTA	1605	CG1	VAL .	A	276	98.492	25.783	-6.962	1.00	24.46 A
5	ATOM	1606	CG2	VAL.	Α	276	96.531	24.248	-6.804	1.00	22.55 A
	MOTA	1607	C	VAL .	Α	276	97.990	26.735	-4.275	1.00	27.83 A
	ATOM	1608	0	VAL .	А	276	99.210	26.849	-4.164	1.00	29.55 A
	ATOM	1609	N	ALA			97.148	27.723	-3.990		26.88 A
	ATOM	1610	CA	ALA			97.639	29.023	-3.549		26.50 A
10	ATOM	1611	CB	ALA			96.765	30.126	-4.122		24.49 A
	ATOM	1612	c	ALA			97.740	29.175	-2.035		26.79 A
	ATOM	1613	0	ALA			98.465	30.042	-1.548		28.26 A
	MOTA	1614	N	GLY			97.020	28.343	-1.290		26.17 A
	MOTA	1615	CA	GLY			97.074	28.430	0.159		24.63 A
15	MOTA	1616	С	GLY.			95.971	29.272	0.780		25.52 A
	ATOM	1617	0	GLY.	Α	278	95.793	29.259	1.998	1.00	27.25 A
	ATOM	1618	N	LEU .	Α	279	95.229	29.998	-0.051	1.00	24.94 A
	ATOM	1619	CA	LEU .	Α	279	94.130	30.849	0.408	1.00	25.58 A
	ATOM	1620	CB	LEU	A	279	94.603	32.302	0.522		27.65 A
20	ATOM	1621	CG	LEU		279	95.748	32.631	1.470		29.35 A
20	ATOM	1622		LEU			96.365	33.958	1.075		30.47 A
			CD2								
	ATOM	1623		LEU .			95.232	32.671	2.892		29.70 A
	ATOM	1624	C	LEU			92.987	30.822	-0.605		25.19 A
	MOTA	1625	0	LEU			93.201	30.525	-1.781		25.34 A
25	ATOM	1626	N	PRO .			91.755	31.126	-0.165		23.60 A
	ATOM	1627	CD	PRO .	Α	280	91.306	31.357	1.216	1.00	22.97 A
	MOTA	1628	CA	PRO .	Α	280	90.628	31.133	-1.103	1.00	23.81 A
	ATOM	1629	CB	PRO .	Α	280	89.417	31.338	-0.195	1.00	25.19 A
	ATOM	1630	CG	PRO .	Α	280	89.982	32.041	1.008	1.00	25.48 A
30	ATOM	1631	C	PRO			90.855	32.295	-2.083		26.26 A
	ATOM	1632	ō	PRO			91.632	33.207	-1.792		25.42 A
	ATOM	1633	N	PRO			90.178	32.284	-3.243		26.49 A
	ATOM	1634	CD	PRO			89.182	31.285	-3.651		27.13 A
	ATOM	1635	CA	PRO			90.307	33.316	-4.281		27.25 A
25											
35	ATOM	1636	CB	PRO			89.522	32.727	-5.463		26.75 A
	ATOM	1637	CG	PRO			89.354	31.291	-5.136		25.29 A
	MOTA	1638	С	PRO .			89.817	34.724	-3.954		27.30 A
	MOTA	1639	0	PRO .			90.497	35.709	-4.238		27.67 A
	MOTA	1640	N	PHE	A	282	88.623	34.817	-3.388	1.00	27.79 A
40	MOTA	1641	CA	PHE	Α	282	88.034	36.107	-3.066	1.00	28.37 A
	ATOM	1642	CB	PHE	Α	282	86.563	36.086	-3.467	1.00	27.77 A
	MOTA	1643	CG	PHE	Α	282	86.335	35.557	-4.857	1.00	29.06 A
	ATOM	1644	CD1	PHE	А	282	86.454	36.392	-5.965	1.00	28.74 A
	ATOM	1645		PHE			86.077	34.207	-5.063		25.80 A
45	ATOM	1646		PHE			86.324	35.887	-7.255		28.50 A
	ATOM	1647	CE2	PHE			85.947	33.695	-6.346		26.04 A
	ATOM	1648	CZ	PHE			86.071	34.535	-7.444		28.02 A
	ATOM	1649	C	PHE			88.184	36.426	-1.589		29.95 A
	MOTA	1650	0	PHE			87.600	35.763	-0.741		32.95 A
50	MOTA	1651	N	ARG			88.977	37.445	-1.285		32.36 A
	ATOM	1652	CA	ARG			89.215	37.843	0.100		33.06 A
	MOTA	1653	CB	ARG .			90.622	37.432	0.520		33.69 A
	MOTA	1654	CG	ARG	Α	283	90.990	36.006	0.151	1.00	36.29 A
	ATOM	1655	CD	ARG	Α	283	92.341	35.635	0.727	1.00	38.81 A
55	ATOM	1656	NE	ARG			93.415	36.423	0.133		41.73 A
	ATOM	1657	CZ	ARG			93.783	36.338	-1.142		44.14 A
	ATOM	1658		ARG			93.162	35.497	-1.958		45.19 A
	ATOM	1659		ARG			94.772	37.094	-1.604		44.57 A
	ATOM	1660	C	ARG			89.065	39.353	0.267		32.44 A
	ATOM	1000	C	ANG	r	203	09.003		0.20/	1.00	32.44 A

	ATOM	1661	0	ARG	Α	283	89.429	40.118	-0.624	1.00 31.91 A
	MOTA	1662	N	ALA	Α	284	88.527	39.777	1.406	1.00 33.21 A
	MOTA	1663	CA	ALA	Α	284	88.348	41.199	1.682	1.00 32.82 A
	ATOM	1664	CB	ALA			87.265	41.777	0.782	1.00 32.40 A
5	ATOM	1665	C	ALA			88.004	41.445	3.147	1.00 32.98 A
	ATOM	1666	ŏ	ALA			87,779	40.502	3.913	1.00 32.53 A
	ATOM	1667				285	87.961	42.723	3.520	1.00 32.60 A
			N							
	ATOM	1668	CA	GLY			87.666	43.112	4.887	1.00 30.00 A
	ATOM	1669	C	GLY			86.355	42.637	5.486	1.00 29.37 A
10	MOTA	1670	0	GLY			86.287	42.366	6.685	1.00 29.35 A
	MOTA	1671	N	ASN	Α	286	85.302	42.547	4.685	1.00 28.99 A
	ATOM	1672	CA	ASN	Α	286	84.024	42.097	5.226	1.00 29.58 A
	MOTA	1673	CB	ASN	Α	286	83.238	43.281	5.801	1.00 29.54 A
	ATOM	1674	CG	ASN	Α	286	82.958	44.356	4.764	1.00 29.60 A
15	ATOM	1675		ASN			82.350	44.092	3.720	1.00 26.48 A
	ATOM	1676		ASN			83.400	45.575	5.049	1.00 25.96 A
	ATOM	1677	С	ASN			83.196	41.378	4.182	1.00 30.16 A
	ATOM	1678	ō	ASN			83.551	41.357	3.004	1.00 31.70 A
										1.00 31.70 A
20	ATOM	1679	N	GLU			82.084	40.796	4.613	
20	MOTA	1680	CA	GLU			81.225	40.051	3.699	1.00 32.53 A
	MOTA	1681	CB	GLU		287	79.943	39.600	4.397	1.00 35.66 A
	MOTA	1682	CG	GLU			80.168	38.813	5.666	1.00 43.05 A
	MOTA	1683	CD	GLU			79.138	37.707	5.856	1.00 47.79 A
	MOTA	1684		GLU			77.933	37.959	5.616	1.00 49.01 A
25	MOTA	1685	OE2	GLU	Α	287	79.539	36.588	6.256	1.00 48.82 A
	MOTA	1686	C	GLU	Α	287	80.853	40.837	2.457	1.00 30.19 A
	MOTA	1687	0	GLU	Α	287	80.986	40.332	1.343	1.00 30.33 A
	MOTA	1688	N	TYR	Α	288	80.385	42.066	2.653	1.00 29.13 A
	ATOM	1689	CA	TYR	А	288	79.972	42.922	1.541	1.00 27.98 A
30	ATOM	1690	CB	TYR	А	288	79.573	44.320	2.034	1.00 26.59 A
	ATOM	1691	CG	TYR			79.080	45.217	0.917	1.00 26.43 A
	ATOM	1692		TYR			77.799	45.060	0.385	1.00 28.06 A
	ATOM	1693		TYR			77.350	45.854	-0.675	1.00 28.72 A
	ATOM	1694	CD2	TYR			79.905	46.196	0.363	1.00 27.24 A
25										
35	MOTA	1695	CE2	TYR			79.470	46.994	-0.697	1.00 28.55 A
	MOTA	1696	CZ	TYR			78.192	46.814	-1.211	1.00 29.91 A
	MOTA	1697	OH	TYR			77.765	47.571	-2.275	1.00 30.53 A
	MOTA	1698	С	TYR			81.057	43.068	0.487	1.00 25.84 A
	MOTA	1699	0	TYR			80.790	42.940	-0.701	1.00 27.88 A
40	MOTA	1700	N	LEU	Α	289	82.279	43.344	0.919	1.00 24.24 A
	MOTA	1701	CA	LEU	Α	289	83.382	43.495	-0.018	1.00 26.60 A
	ATOM	1702	CB	LEU	Α	289	84.662	43.919	0.713	1.00 25.15 A
	MOTA	1703	CG	LEU	Α	289	85.005	45.411	0.817	1.00 27.82 A
	ATOM	1704	CD1	LEU	Α	289	83.830	46.277	0.354	1.00 27.32 A
45	MOTA	1705	CD2	LEU	Α	289	85.404	45.727	2.251	1.00 25.62 A
	ATOM	1706	C	LEU			83.622	42.184	-0.736	1.00 27.45 A
	ATOM	1707	ō	LEU			83.901	42.157	-1.933	1.00 30.18 A
	ATOM	1708	N	ILE			83.520	41.093	0.009	1.00 28.11 A
	ATOM	1709	CA	ILE			83.726	39.770	-0.551	1.00 28.84 A
50										
50	ATOM	1710	CB	ILE			83.565	38.710	0.545	1.00 29.67 A
	MOTA	1711	CG2	ILE			83.450	37.331	-0.071	1.00 31.47 A
	MOTA	1712		ILE			84.756	38.802	1.504	1.00 29.26 A
	MOTA	1713		ILE			84.604	37.995	2.779	1.00 27.48 A
	MOTA	1714	C	ILE			82.727	39.530	-1.676	1.00 27.99 A
55	MOTA	1715	0	ILE	Α	290	83.090	39.110	-2.775	1.00 26.63 A
	MOTA	1716	N	PHE	Α	291	81.464	39.824	-1.406	1.00 28.54 A
	MOTA	1717	CA	PHE	Α	291	80.432	39.638	-2.407	1.00 27.14 A
	ATOM	1718	CB	PHE			79.066	39.945	-1.807	1.00 28.37 A
	ATOM	1719	CG	PHE	Α	291	78.674	39.024	-0.688	1.00 30.37 A

	MOTA	1720		PHE			79.283	37.778	-0.543	1.00 30.07 A
	MOTA	1721	CD2	PHE			77.658	39.377	0.194	1.00 29.74 A
	MOTA	1722	CE1	PHE	Α	291	78.885	36.897	0.463	1.00 32.11 A
	MOTA	1723	CE2	PHE	Α	291	77.253	38.502	1.202	1.00 32.76 A
5	ATOM	1724	CZ	PHE	Α	291	77.867	37.259	1.336	1.00 32.01 A
	MOTA	1725	C	PHE	Α	291	80.690	40.525	-3.618	1.00 27.79 A
	ATOM	1726	0	PHE	Α	291	80.434	40.124	-4.755	1.00 26.52 A
	ATOM	1727	N	GLN	Α	292	81.200	41.730	-3.384	1.00 27.05 A
	ATOM	1728	CA	GLN			81.478	42.613	-4.503	1.00 27.48 A
10	ATOM	1729	CB	GLN			82.072	43.945	-4.037	1.00 27.80 A
	ATOM	1730	CG	GLN			81.041	44.984	-3.651	1.00 30.50 A
	ATOM	1731	CD	GLN			81.630	46.381	-3.565	1.00 31.30 A
	ATOM	1732		GLN			82.519	46.644	-2.762	1.00 33.17 A
	ATOM	1733		GLN			81.133	47.284	-4.399	1.00 32.86 A
15	ATOM	1734	C	GLN			82.442	41.934	-5.460	1.00 32.00 A
15	ATOM	1735	ō	GLN			82.186	41.883	-6.664	1.00 28.03 A
	ATOM	1736	N	LYS			83.539	41.402	-4.924	1.00 24.08 A
		1737		LYS			84.542	40.739	-5.751	1.00 24.00 A
	ATOM	1738	CA	LYS			85.752	40.739	-4.901	1.00 24.43 A
20	ATOM		CB							
20	ATOM	1739	CG	LYS			86.456	41.580	-4.319	1.00 28.24 A
	ATOM	1740	CD	LYS			87.750	41.213	-3.608	1.00 30.60 A
	MOTA	1741	CE	LYS			88.555	42.468	-3.273	1.00 32.23 A
	MOTA	1742	NZ	LYS			89.849	42.170	-2.591	1.00 32.86 A
	MOTA	1743	C	LYS			84.008	39.500	-6.472	1.00 25.06 A
25	MOTA	1744	0	LYS			84.350	39.236	-7.628	1.00 24.96 A
	MOTA	1745	N	ILE			83.163	38.740	-5.793	1.00 24.33 A
	ATOM	1746	CA	ILE			82.593	37.552	-6.399	1.00 24.46 A
	MOTA	1747	CB	ILE			81.725	36.800	-5.385	1.00 22.52 A
	MOTA	1748	CG2	ILE	Α	294	80.837	35.783	-6.093	1.00 23.14 A
30	MOTA	1749	CG1	ILE	Α	294	82.632	36.141	-4.345	1.00 21.54 A
	ATOM	1750	CD1	ILE	Α	294	81.892	35.535	-3.175	1.00 19.38 A
	ATOM	1751	С	ILE	Α	294	81.761	37.885	-7.639	1.00 27.01 A
	ATOM	1752	0	ILE	Α	294	81.967	37.303	-8.704	1.00 23.93 A
	ATOM	1753	N	ILE	Α	295	80.830	38.828	-7.513	1.00 29.79 A
35	ATOM	1754	CA	ILE	Α	295	79.983	39.168	-8.653	1.00 32.98 A
	ATOM	1755	CB	ILE	А	295	78.767	40.004	-8.228	1.00 33.96 A
	ATOM	1756	CG2	ILE	А	295	77.980	39.246	-7.174	1.00 36.23 A
	ATOM	1757		ILE			79.216	41.358	-7.682	1.00 35.79 A
	ATOM	1758		ILE			78.062	42.266	-7.300	1.00 37.79 A
40	ATOM	1759	c	ILE			80.729	39.898	-9.757	1.00 33.17 A
	ATOM	1760	ō	ILE			80.212		-10.862	1.00 34.06 A
	ATOM	1761	N	LYS			81.946	40.333	-9.462	1.00 33.65 A
	ATOM	1762	CA	LYS			82.747		-10.468	1.00 34.81 A
	ATOM	1763	CB	LYS			83.353	42.293	-9.895	1.00 38.05 A
45	ATOM	1764	CG	LYS			82.353	43.427	-9.714	1.00 40.12 A
75	ATOM	1765	CD	LYS			83.070	44.736	-9.401	1.00 40.12 A
	ATOM	1766	CE	LYS			82.191	45.939	-9.731	1.00 44.01 A
	ATOM	1767	NZ	LYS			82.972	47.209	-9.833	1.00 40.00 A
	ATOM	1768		LYS			83.851		-10.945	1.00 47.40 A
50			C							
30	ATOM	1769	0	LYS			84.622		-11.847	1.00 33.48 A
	MOTA	1770	N	LEU			83.907		-10.333	1.00 33.82 A
	ATOM	1771	CA	LEU			84.904		-10.663	1.00 32.06 A
	MOTA	1772	СВ	LEU			84.716		-12.110	1.00 32.43 A
	MOTA	1773	CG	LEU			85.452		-12.538	1.00 33.09 A
55	MOTA	1774		LEU			84.959		-11.697	1.00 31.88 A
	MOTA	1775		LEU			85.206		-14.025	1.00 32.51 A
	MOTA	1776	C	LEU			86.275		-10.476	1.00 32.23 A
	MOTA	1777	0	LEU			87.180		-11.278	1.00 32.08 A
	MOTA	1778	N	GLU	Α	298	86.424	39.267	-9.395	1.00 33.56 A

	MOTA	1779	CA	GLU			87.682	39.936	-9.110		35.66 A
	MOTA	1780	CB	GLU			87.405	41.274	-8.428		38.03 A
	MOTA	1781	CG	GLU	Α	298	88.641	42.125	-8.236	1.00	42.97 A
	MOTA	1782	CD	GLU	Α	298	88.383	43.313	-7.338	1.00	46.19 A
5	ATOM	1783	OE1	GLU	Α	298	87.412	44.055	-7.602	1.00	48.41 A
	MOTA	1784	OE2	GLU	Α	298	89.153	43.504	-6.369	1.00	48.44 A
	MOTA	1785	C	GLU	Α	298	88.644	39.117	-8.245	1.00	34.35 A
	ATOM	1786	0	GLU			88.508	39.065	-7.021	1.00	35.64 A
	ATOM	1787	N	TYR			89.611	38.478	-8.894		32.46 A
10	ATOM	1788	CA	TYR			90.624	37.678	-8.208		30.71 A
	ATOM	1789	CB	TYR			90.031	36.367	-7.672		26.01 A
	ATOM	1790	CG	TYR			89.874	35.300	-8.730		26.77 A
	ATOM	1791		TYR			88.871	35.390	-9.699		26.60 A
	ATOM	1792		TYR			88.768		-10.724		26.10 A
15	ATOM	1793	CD2	TYR			90.770	34.236	-8.807		22.56 A
13	ATOM	1794		TYR			90.677	33.291	-9.822		24.59 A
			CE2								
	MOTA	1795	CZ	TYR			89.674		-10.781		26.34 A
	MOTA	1796	OH	TYR			89.578		-11.791		22.44 A
	MOTA	1797	С	TYR			91.720	37.374	-9.229		30.95 A
20	MOTA	1798	0	TYR			91.528		-10.425		28.80 A
	MOTA	1799	N	ASP			92.865	36.891	-8.764		33.38 A
	MOTA	1800	CA	ASP		300	93.954	36.582	-9.680		36.47 A
	MOTA	1801	CB	ASP	Α	300	94.782	37.845	-9.931		42.34 A
	MOTA	1802	CG	ASP	Α	300	95.014	38.644	-8.666	1.00	46.20 A
25	MOTA	1803	OD1	ASP	Α	300	95.607	38.085	-7.719	1.00	49.27 A
	ATOM	1804	OD2	ASP	Α	300	94.599	39.826	-8.615	1.00	49.25 A
	MOTA	1805	C	ASP	Α	300	94.848	35.444	-9.188	1.00	35.61 A
	MOTA	1806	0	ASP	Α	300	94.857	35.113	-8.002	1.00	34.48 A
	ATOM	1807	N	PHE	Α	301	95.602	34.854	-10.111	1.00	35.02 A
30	ATOM	1808	CA	PHE		301	96.477	33.737	-9.781		35.94 A
	MOTA	1809	CB	PHE		301	96.501		-10.909		34.28 A
	ATOM	1810	CG	PHE			95.156		-11.301		32.40 A
	ATOM	1811		PHE			94.358		-12.205		30.50 A
	ATOM	1812	CD2	PHE		301	94.708		-10.803		31.83 A
35	ATOM	1813	CE1	PHE			93.131		-12.617		31.48 A
33	ATOM	1814	CE2	PHE			93.484		-11.206		31.37 A
	ATOM	1815	CZ	PHE			92.695		-12.114		31.44 A
	ATOM	1816	C	PHE		301	97.916	34.134	-9.524		38.11 A
			Ö	PHE							39.06 A
40	ATOM	1817					98.458		-10.196		
40	MOTA	1818	N	PRO			98.559	33.498	-8.535		40.47 A
	MOTA	1819	CD	PRO			98.053	32.554	-7.524		41.16 A
	MOTA	1820	CA	PRO		302	99.955	33.843	-8.277		41.88 A
	MOTA	1821	CB	PRO			100.248	33.131	-6.963		42.01 A
	MOTA	1822	CG	PRO			99.328	31.947	-7.001		41.79 A
45	MOTA	1823	С	PRO			100.721	33.265	-9.458		44.54 A
	MOTA	1824	0	PRO		302	100.263		-10.082		44.30 A
	MOTA	1825	N	GLU			101.874	33.843	-9.770		47.35 A
	MOTA	1826	CA	GLU	Α	303	102.667	33.395	-10.912	1.00	50.51 A
	MOTA	1827	CB	GLU	Α	303	103.859	34.337	-11.105	1.00	53.23 A
50	MOTA	1828	CG	GLU	Α	303	104.431	34.376	-12.520	1.00	56.85 A
	MOTA	1829	CD	GLU	Α	303	103.976	35.600	-13.314	1.00	59.62 A
	MOTA	1830	OE1	GLU	Α	303	104.508	35.819	-14.424	1.00	60.43 A
	ATOM	1831		GLU		303	103.088		-12.834		60.45 A
	ATOM	1832	C	GLU		303	103.173		-10.829		50.70 A
55	ATOM	1833	o	GLU		303	103.692		-11.815		52.21 A
	ATOM	1834	N	ALA		304	103.018	31.309	-9.672		49.61 A
	ATOM	1835	CA	ALA		304	103.495	29.933	-9.488		49.10 A
	ATOM	1836	CB	ALA		304	104.077	29.779	-8.082		48.82 A
	ATOM	1837	CB	ALA			102.422	28.869	-9.713		47.90 A
	MIUN	TO 2 /	-	мим	м	204	102.422	40.009	-3.113	1.00	3/.30 A

	MOTA	1838	0	ALA			102.703	27.666 -9.719	1.00 49.41 A
	MOTA	1839	N	PHE			101.192	29.322 -9.899	1.00 44.69 A
	MOTA	1840	CA	PHE			100.053	28.440 -10.089	1.00 40.05 A
	MOTA	1841	CB	PHE	Α	305	98.809	29.301 -10.299	1.00 39.69 A
5	ATOM	1842	CG	PHE	А	305	97.568	28.729 -9.697	1.00 37.21 A
	ATOM	1843	CD1	PHE	А	305	96.824	27.775 -10.379	1.00 35.36 A
	ATOM	1844		PHE			97.133	29.157 -8.445	1.00 37.52 A
	ATOM	1845		PHE			95.658	27.255 -9.825	1.00 34.59 A
	ATOM	1846		PHE			95.963	28.641 -7.880	1.00 37.01 A
10		1847		PHE			95.226		1.00 37.01 A
10	ATOM		CZ						
	MOTA	1848	С	PHE			100.197	27.435 -11.230	1.00 37.65 A
	MOTA	1849	0	PHE			100.364	27.814 -12.389	1.00 36.24 A
	MOTA	1850	N	PHE			100.120	26.150 -10.892	1.00 35.64 A
	MOTA	1851	CA	PHE	Α	306	100.219	25.081 -11.884	1.00 32.40 A
15	MOTA	1852	CB	PHE	Α	306	99.781	23.749 -11.268	1.00 29.92 A
	ATOM	1853	CG	PHE	Α	306	100.412	23.456 -9.926	1.00 28.24 A
	MOTA	1854	CD1	PHE	А	306	101.796	23.457 -9.770	1.00 27.43 A
	ATOM	1855	CD2	PHE	А	306	99.617	23.173 -8.816	1.00 28.59 A
	ATOM	1856		PHE		306	102.380	23.181 -8.526	1.00 29.55 A
20	ATOM	1857	CE2	PHE			100.188	22.895 -7.566	1.00 29.06 A
20	ATOM	1858	CZ	PHE			101.575	22.901 -7.422	1.00 29.51 A
	ATOM	1859	C	PHE			99.296	25.452 -13.047	1.00 29.31 A
		1860							
	MOTA		0	PHE			98.087	25.625 -12.861	1.00 34.51 A
	MOTA	1861	N	PRO			99.856	25.587 -14.262	1.00 31.43 A
25	ATOM	1862	CD	PRO			101.272	25.327 -14.569	1.00 30.74 A
	MOTA	1863	CA	PRO			99.128	25.947 -15.485	1.00 29.54 A
	MOTA	1864	CB	PRO			100.158	25.700 -16.579	1.00 29.48 A
	MOTA	1865	CG	PRO			101.437	26.032 -15.895	1.00 30.81 A
	MOTA	1866	C	PRO	Α	307	97.826	25.193 -15.743	1.00 29.74 A
30	MOTA	1867	0	PRO	Α	307	96.795	25.804 -16.022	1.00 31.08 A
	ATOM	1868	N	LYS	Α	308	97.867	23.870 -15.660	1.00 28.47 A
	ATOM	1869	CA	LYS	Α	308	96.672	23.086 -15.904	1.00 27.92 A
	ATOM	1870	CB	LYS	А	308	97.044	21.619 -16.114	1.00 28.70 A
	ATOM	1871	CG	LYS	А	308	97.696	21.405 -17.460	1.00 30.04 A
35	ATOM	1872	CD	LYS			98.310	20.029 -17.595	1.00 33.76 A
	ATOM	1873	CE	LYS			99.106	19.926 -18.888	1.00 33.22 A
	ATOM	1874	NZ	LYS			99.897	18.663 -18.948	1.00 36.67 A
	ATOM	1875	C	LYS			95.632	23.247 -14.800	1.00 26.85 A
	ATOM	1876	0	LYS			94.433	23.170 -15.060	1.00 25.34 A
40									
40	ATOM	1877	N	ALA			96.084	23.480 -13.574	1.00 24.70 A
	ATOM	1878	CA	ALA			95.145	23.685 -12.486	1.00 24.41 A
	MOTA	1879	CB	ALA			95.855	23.652 -11.146	1.00 22.65 A
	MOTA	1880	C	ALA			94.523	25.051 -12.712	1.00 26.56 A
	MOTA	1881	0	ALA			93.327	25.238 -12.493	1.00 28.91 A
45	MOTA	1882	N	ARG	Α	310	95.335	26.011 -13.149	1.00 26.94 A
	MOTA	1883	CA	ARG	Α	310	94.830	27.354 -13.402	1.00 27.56 A
	ATOM	1884	CB	ARG	Α	310	95.961	28.289 -13.864	1.00 28.69 A
	ATOM	1885	CG	ARG	Α	310	95.438	29.584 -14.480	1.00 31.42 A
	ATOM	1886	CD	ARG			96.482	30.676 -14.634	1.00 33.72 A
50	ATOM	1887	NE	ARG			95.881	31.868 -15.233	1.00 37.73 A
	ATOM	1888	CZ	ARG			96.412	33.090 -15.198	1.00 38.44 A
	ATOM	1889		ARG			97.572	33.297 -14.588	1.00 37.72 A
	ATOM	1890		ARG			95.775	34.108 -15.767	1.00 37.72 A
	MOTA	1891	C	ARG			93.743	27.280 -14.473	1.00 26.84 A
55	MOTA	1892	0	ARG			92.678	27.880 -14.344	1.00 26.39 A
	MOTA	1893	N	ASP			94.019	26.524 -15.527	1.00 26.91 A
	MOTA	1894	CA	ASP			93.069	26.369 -16.615	1.00 28.21 A
	ATOM	1895	CB	ASP			93.682	25.504 -17.713	1.00 30.32 A
	MOTA	1896	CG	ASP	Α	311	92.850	25.494 -18.972	1.00 35.68 A

	ATOM	1897		ASP .			91.894	24.691 -19.040		38.27 A	
	MOTA	1898	OD2	ASP .	A	311	93.145	26.302 -19.888	1.00	37.07 A	
	MOTA	1899	C	ASP .	Α	311	91.769	25.748 -16.108	1.00	27.22 A	
	MOTA	1900	0	ASP .	Α	311	90.678	26.205 -16.449	1.00	29.64 A	
5	ATOM	1901	N	LEU .	Α	312	91.886	24.715 -15.285	1.00	24.32 A	
	ATOM	1902	CA	LEU .	A	312	90.708	24.062 -14.728		23.48 A	
	ATOM	1903	CB	LEU .			91.118	22.838 -13.892		21.65 A	
	ATOM	1904	CG	LEU .			90.067	22.228 -12.945		21.40 A	
	ATOM	1905		LEU .			88.789	21.917 -13.694		16.90 A	
10	MOTA	1906		LEU .			90.629	20.960 -12.294		19.67 A	
10	ATOM	1907	C	LEU .			89.899	25.039 -13.871		22.73 A	
										22.73 A 22.02 A	
	ATOM	1908	0	LEU .			88.684	25.141 -14.021			
	MOTA	1909	N	VAL .			90.574	25.754 -12.972		22.12 A	
	MOTA	1910	CA	VAL .			89.897	26.715 -12.108		21.16 A	
15	MOTA	1911	CB	VAL .			90.893	27.440 -11.167		23.49 A	
	MOTA	1912		VAL .			90.221	28.679 -10.534		20.45 A	
	ATOM	1913		VAL .			91.369	26.487 -10.080		21.63 A	
	MOTA	1914	С	VAL .			89.161	27.771 -12.920		22.93 A	
	MOTA	1915	0	VAL .	Α	313	88.051	28.168 -12.566	1.00	21.46 A	
20	ATOM	1916	N	GLU .	Α	314	89.784	28.235 -14.001	1.00	23.15 A	
	ATOM	1917	CA	GLU .	Α	314	89.156	29.252 -14.832	1.00	25.95 A	
	ATOM	1918	CB	GLU .	Α	314	90.127	29.762 -15.900	1.00	28.61 A	
	ATOM	1919	CG	GLU .	A	314	91.319	30.523 -15.350	1.00	32.73 A	
	ATOM	1920	CD	GLU .			92.205	31.059 -16.453		35.94 A	
25	ATOM	1921		GLU .			92.188	30.467 -17.554		40.67 A	
	ATOM	1922	OE2	GLU .			92.923	32.059 -16.225		37.73 A	
	ATOM	1923	c	GLU .			87.891	28.742 -15.505		24.64 A	
	ATOM	1924	Ö	GLU .			87.030	29.528 -15.892		24.01 A	
	ATOM	1925	N	LYS .			87.775	27.428 -15.654		23.67 A	
30	ATOM	1926	CA	LYS .		315	86.588	26.874 -16.278		23.15 A	
30											
	ATOM	1927	CB	LYS .			86.937	25.594 -17.042		24.76 A	
	ATOM	1928	CG	LYS .			87.784	25.845 -18.299		22.90 A	
	MOTA	1929	CD	LYS .			88.223	24.541 -18.929		23.63 A	
	MOTA	1930	CE	LYS .			89.079	24.772 -20.153		23.20 A	
35	MOTA	1931	NZ	LYS .			88.332	25.582 -21.142		29.09 A	
	MOTA	1932	C	LYS .			85.509	26.600 -15.244		23.08 A	
	MOTA	1933	0	LYS .			84.386	26.250 -15.596		23.63 A	
	MOTA	1934	N	LEU .			85.852	26.773 -13.969		21.74 A	
	MOTA	1935	CA	LEU .			84.910	26.547 -12.876		21.89 A	
40	MOTA	1936	CB	LEU .	Α	316	85.569	25.738 -11.760	1.00	20.54 A	
	ATOM	1937	CG	LEU .	Α	316	85.841	24.269 -12.090	1.00	20.69 A	
	ATOM	1938	CD1	LEU .	Α	316	86.600	23.611 -10.947	1.00	17.08 A	
	ATOM	1939	CD2	LEU .	A	316	84.514	23.558 -12.336	1.00	19.15 A	
	ATOM	1940	С	LEU .	A	316	84.404	27.860 -12.312	1.00	23.66 A	
45	ATOM	1941	0	LEU .			83.215	28.005 -12.013		25.40 A	
	ATOM	1942	N	LEU .		317	85.310	28.816 -12.149		24.48 A	
	ATOM	1943	CA	LEU .			84.933	30.121 -11.637		25.52 A	
	ATOM	1944	CB	LEU .			86.123	30.793 -10.936		24.23 A	
	ATOM	1945	CG	LEU .			86.656	30.035 -9.719		21.22 A	
50				LEU .			87.718				
30	MOTA	1946				317		30.859 -9.015			
	ATOM	1947		LEU .			85.515	29.730 -8.773		21.36 A	
	MOTA	1948	С	LEU .			84.459	30.953 -12.815		26.00 A	
	MOTA	1949	0	LEU .			85.148	31.856 -13.286		28.02 A	
	MOTA	1950	N	VAL .		318	83.272	30.611 -13.293		27.50 A	
55	MOTA	1951	CA	VAL .			82.643	31.286 -14.421		28.43 A	
	MOTA	1952	CB	VAL .			82.365	30.280 -15.558	1.00	28.13 A	
	ATOM	1953		VAL .			81.624	30.953 -16.694	1.00	29.20 A	
	ATOM	1954	CG2	VAL .	Α	318	83.677	29.689 -16.045	1.00	27.12 A	
	ATOM	1955	C	VAL .	Α	318	81.331	31.842 -13.896	1.00	29.21 A	

	ATOM	1956	0	VAL			80.559	31.120 -13.255	1.00 30.06 A
	MOTA	1957	N	LEU	Α	319	81.082	33.121 -14.150	1.00 29.94 A
	MOTA	1958	CA	LEU	Α	319	79.858	33.758 -13.671	1.00 30.57 A
	ATOM	1959	CB	LEU	Α	319	79.808	35.214 -14.133	1.00 32.89 A
5	ATOM	1960	CG	LEU	А	319	80.908	36.115 -13.553	1.00 35.26 A
	MOTA	1961		LEU			80.741	37.551 -14.059	1.00 34.63 A
	ATOM	1962		LEU			80.835	36.078 -12.028	1.00 34.01 A
	ATOM	1963	C	LEU			78.598	33.029 -14.117	1.00 30.01 A
	ATOM	1964	0	LEU			77.704	32.768 -13.316	1.00 30.01 A
10									
10	MOTA	1965	N	ASP			78.527	32.695 -15.397	1.00 30.13 A
	MOTA	1966	CA	ASP			77.362	31.996 -15.919	1.00 29.97 A
	MOTA	1967	CB	ASP			77.393	31.981 -17.444	1.00 32.99 A
	MOTA	1968	CG	ASP	Α	320	76.116	31.435 -18.040	1.00 36.86 A
	MOTA	1969	OD1	ASP	Α	320	75.495	30.548 -17.412	1.00 38.81 A
15	ATOM	1970	OD2	ASP	Α	320	75.739	31.883 -19.142	1.00 38.26 A
	ATOM	1971	C	ASP	Α	320	77.373	30.569 -15.402	1.00 28.61 A
	ATOM	1972	0	ASP	А	320	78.244	29.786 -15.758	1.00 28.87 A
	ATOM	1973	N	ALA			76.398	30.233 -14.566	1.00 28.88 A
	ATOM	1974	CA	ALA			76.311	28.897 -13.980	1.00 28.04 A
20	ATOM	1975	CB	ALA			75.156	28.842 -12.990	1.00 25.04 A
20	ATOM	1976	C	ALA			76.151	27.794 -15.021	1.00 27.83 A
	MOTA	1977	0	ALA			76.500	26.643 -14.773	1.00 27.26 A
	MOTA	1978	N	THR			75.632	28.150 -16.190	1.00 27.45 A
	MOTA	1979	CA	THR			75.413	27.167 -17.243	1.00 27.18 A
25	MOTA	1980	CB	THR			74.294	27.615 -18.191	1.00 26.99 A
	ATOM	1981		THR			74.739	28.753 -18.940	1.00 27.15 A
	MOTA	1982	CG2	THR	Α	322	73.045	27.997 -17.399	1.00 23.11 A
	MOTA	1983	С	THR	Α	322	76.654	26.909 -18.077	1.00 28.31 A
	MOTA	1984	0	THR	Α	322	76.605	26.133 -19.027	1.00 28.80 A
30	ATOM	1985	N	LYS	Α	323	77.769	27.546 -17.727	1.00 28.30 A
	ATOM	1986	CA	LYS	А	323	78.990	27.348 -18.491	1.00 28.51 A
	ATOM	1987	CB	LYS			79.392	28.651 -19.172	1.00 30.27 A
	ATOM	1988	CG	LYS			78.305	29.160 -20.095	1.00 35.72 A
	ATOM	1989	CD	LYS			78.839	30.081 -21.170	1.00 37.65 A
35	ATOM	1990	CE	LYS			77.722	30.472 -22.131	1.00 37.65 A
33									
	ATOM	1991	NZ	LYS			77.088	29.263 -22.733	1.00 40.41 A
	MOTA	1992	С	LYS			80.154	26.799 -17.683	1.00 28.68 A
	MOTA	1993	0	LYS			81.298	26.847 -18.119	1.00 29.54 A
	MOTA	1994	N	ARG			79.866	26.271 -16.503	1.00 27.43 A
40	MOTA	1995	CA	ARG			80.921	25.709 -15.684	1.00 25.01 A
	ATOM	1996	CB	ARG	Α	324	80.559	25.800 -14.205	1.00 22.81 A
	MOTA	1997	CG	ARG	Α	324	80.489	27.223 -13.715	1.00 21.68 A
	ATOM	1998	CD	ARG	Α	324	80.036	27.315 -12.277	1.00 20.65 A
	MOTA	1999	NE	ARG	Α	324	79.655	28.689 -11.971	1.00 21.18 A
45	ATOM	2000	CZ	ARG	Α	324	78.645	29.029 -11.180	1.00 19.20 A
	ATOM	2001	NH1	ARG			77.909	28.093 -10.598	1.00 19.05 A
	ATOM	2002		ARG			78.349	30.307 -11.004	1.00 19.45 A
	ATOM	2003	C	ARG			81.161	24.264 -16.073	1.00 24.64 A
	ATOM	2004	Ö	ARG			80.219	23.501 -16.290	1.00 23.78 A
50	ATOM	2005	N	LEU			82.433	23.902 -16.177	1.00 23.76 A
50									
	MOTA	2006	CA	LEU			82.809	22.541 -16.526	1.00 25.53 A
	MOTA	2007	CB	LEU			84.336	22.422 -16.558	1.00 25.18 A
	ATOM	2008	CG	LEU			84.995	21.178 -17.149	1.00 25.63 A
	MOTA	2009		LEU		325	84.541	20.949 -18.590	1.00 25.39 A
55	MOTA	2010		LEU			86.500	21.364 -17.087	1.00 23.10 A
	MOTA	2011	C	LEU	Α	325	82.224	21.610 -15.466	1.00 25.01 A
	MOTA	2012	0	LEU		325	82.449	21.809 -14.278	1.00 23.81 A
	MOTA	2013	N	GLY	Α	326	81.450	20.616 -15.900	1.00 26.41 A
	ATOM	2014	CA	GLY	Α	326	80.850	19.683 -14.964	1.00 26.13 A

	ATOM	2015	Ç	GLY			79.338	19.771 -14.835	1.00 29.31 A
	ATOM	2016	0	GLY			78.697	18.795 -14.444	1.00 31.67 A
	MOTA	2017	N	CYS			78.753	20.918 -15.162	1.00 29.49 A
	ATOM	2018	CA	CYS			77.308	21.073 -15.042	1.00 31.91 A
5	ATOM	2019	CB	CYS	Α	327	76.935	22.556 -14.982	1.00 31.78 A
	ATOM	2020	SG	CYS	Α	327	77.084	23.397 -16.552	1.00 38.33 A
	ATOM	2021	C	CYS	Α	327	76.539	20.385 -16.175	1.00 32.76 A
	ATOM	2022	0	CYS	Α	327	77.096	20.069 -17.228	1.00 32.18 A
	ATOM	2023	N	GLU	Α	328	75.248	20.175 -15.952	1.00 33.60 A
10	ATOM	2024	CA	GLU	Α	328	74.400	19.497 -16.921	1.00 36.82 A
	ATOM	2025	CB	GLU	А	328	72.951	19.479 -16.408	1.00 41.60 A
	ATOM	2026	CG	GLU			72.845	19.437 -14.863	1.00 48.96 A
	ATOM	2027	CD	GLU			72.000	18.279 -14.321	1.00 51.75 A
	ATOM	2028		GLU			72.393	17.103 -14.509	1.00 52.77 A
15	ATOM	2029		GLU			70.948	18.550 -13.696	1.00 52.29 A
	ATOM	2030	c	GLU			74.466	20.120 -18.317	1.00 35.83 A
	ATOM	2031	o	GLU			74.618	19.412 -19.318	1.00 34.85 A
	ATOM	2032	N	GLU			74.370	21.443 -18.378	1.00 33.75 A
	ATOM	2032	CA	GLU			74.399	22.146 -19.650	1.00 33.73 A
20	ATOM	2033	CB	GLU			74.153	23.640 -19.439	1.00 32.37 A
20	ATOM	2034	CG	GLU			72.898	23.972 -18.640	1.00 34.70 A
	ATOM	2036	CD	GLU			73.017	23.589 -17.172	1.00 38.53 A
	MOTA	2037		GLU			74.048	23.926 -16.548	1.00 44.03 A
2.5	ATOM	2038		GLU			72.080	22.958 -16.636	1.00 44.74 A
25	ATOM	2039	С	GLU			75.711	21.947 -20.399	1.00 30.96 A
	ATOM	2040	0	GLU			75.757	22.114 -21.617	1.00 28.90 A
	MOTA	2041	N	MET			76.773	21.605 -19.673	1.00 29.20 A
	MOTA	2042	CA	MET			78.075	21.379 -20.291	1.00 27.90 A
	MOTA	2043	CB	MET			79.190	22.010 -19.455	1.00 30.57 A
30	ATOM	2044	CG	MET			79.189	23.536 -19.446	1.00 32.33 A
	MOTA	2045	SD	MET			79.488	24.269 -21.070	1.00 36.55 A
	ATOM	2046	CE	MET			81.257	24.001 -21.239	1.00 35.61 A
	MOTA	2047	C	MET			78.319	19.883 -20.443	1.00 27.32 A
	ATOM	2048	0	MET	Α	330	79.452	19.436 -20.606	1.00 25.82 A
35	ATOM	2049	N	GLU	Α	331	77.232	19.122 -20.365	1.00 25.18 A
	ATOM	2050	CA	GLU	Α	331	77.246	17.677 -20.526	1.00 24.56 A
	ATOM	2051	CB	GLU	Α	331	77.922	17.295 -21.848	1.00 23.55 A
	MOTA	2052	CG	GLU	Α	331	77.395	18.099 -23.030	1.00 25.42 A
	MOTA	2053	CD	GLU	Α	331	75.867	18.176 -23.082	1.00 28.50 A
40	ATOM	2054	OE1	GLU	Α	331	75.338	19.094 -23.750	1.00 31.00 A
	ATOM	2055	OE2	GLU	Α	331	75.190	17.323 -22.467	1.00 30.18 A
	ATOM	2056	C	GLU	Α	331	77.804	16.834 -19.396	1.00 24.55 A
	ATOM	2057	0	GLU	Α	331	78.327	15.745 -19.629	1.00 25.02 A
	ATOM	2058	N	GLY	Α	332	77.692	17.339 -18.172	1.00 22.83 A
45	ATOM	2059	CA	GLY	Α	332	78.098	16.564 -17.017	1.00 20.57 A
	ATOM	2060	C	GLY			79.541	16.408 -16.606	1.00 20.81 A
	ATOM	2061	o	GLY			80.430	17.167 -16.999	1.00 19.36 A
	ATOM	2062	N	TYR			79.753	15.374 -15.801	1.00 20.19 A
	ATOM	2063	CA	TYR			81.053	15.056 -15.243	1.00 20.12 A
50	ATOM	2064	CB	TYR			80.860	14.127 -14.052	1.00 20.05 A
50	ATOM	2065	CG	TYR			80.483	14.902 -12.828	1.00 21.40 A
	ATOM	2066		TYR			81.464	15.367 -11.956	1.00 21.40 A
	ATOM	2066		TYR			81.141	16.181 -10.878	1.00 22.85 A
	ATOM	2067		TYR			79.160		1.00 22.91 A
55				TYR			78.827	15.266 -12.590 16.082 -11.518	1.00 21.24 A 1.00 22.71 A
23	MOTA	2069							
	ATOM	2070	CZ	TYR			79.827	16.535 -10.670	1.00 21.44 A
	ATOM	2071	OH	TYR			79.522	17.358 -9.621	1.00 24.72 A
	ATOM	2072	C	TYR			82.076	14.484 -16.192	1.00 20.38 A
	MOTA	2073	0	TYR	Α	333	83.277	14.533 -15.910	1.00 18.82 A

	ATOM	2074	N	GLY	Α	334	81.610	13.942 -17.313	1.00 20.41 A
	ATOM	2075	CA	GLY	Α	334	82.534	13.378 -18.280	1.00 20.48 A
	ATOM	2076	С	GLY	Α	334	83.611	14.367 -18.693	1.00 20.12 A
	ATOM	2077	0	GLY			84.808	14.105 -18.539	1.00 21.13 A
5	ATOM	2078	N	PRO			83.216	15.524 -19.230	1.00 19.75 A
	ATOM	2079	CD	PRO			81.872	15.899 -19.699	1.00 19.25 A
	ATOM	2080	CA	PRO			84.218	16.512 -19.644	1.00 19.66 A
	ATOM	2081	CB	PRO			83.366	17.644 -20.212	1.00 17.92 A
10	ATOM	2082	CG	PRO			82.184	16.901 -20.784	1.00 19.24 A
10	MOTA	2083	С	PRO			85.115	16.967 -18.495	1.00 19.62 A
	MOTA	2084	0	PRO			86.315	17.154 -18.679	1.00 21.87 A
	MOTA	2085	N	LEU			84.538	17.131 -17.307	1.00 19.91 A
	MOTA	2086	CA	LEU			85.312	17.576 -16.147	1.00 19.06 A
	MOTA	2087	CB	LEU			84.406	17.767 -14.914	1.00 18.05 A
15	MOTA	2088	CG	LEU	Α	336	85.073	18.119 -13.571	1.00 18.25 A
	ATOM	2089	CD1	LEU	Α	336	86.049	19.280 -13.746	1.00 15.57 A
	MOTA	2090	CD2	LEU	Α	336	84.009	18.473 -12.538	1.00 15.31 A
	ATOM	2091	С	LEU	Α	336	86.424	16.594 -15.832	1.00 17.85 A
	ATOM	2092	0	LEU	Α	336	87.582	16.986 -15.690	1.00 17.14 A
20	ATOM	2093	N	LYS	А	337	86.075	15.317 -15.732	1.00 17.96 A
	ATOM	2094	CA	LYS			87.061	14.289 -15.438	1.00 19.15 A
	ATOM	2095	CB	LYS			86.352	12.966 -15.134	1.00 21.53 A
	ATOM	2096	CG	LYS			85.571	13.025 -13.821	1.00 25.58 A
	ATOM	2097	CD	LYS			84.484	11.956 -13.715	1.00 26.69 A
25	ATOM	2098	CE	LYS			85.063	10.566 -13.571	1.00 29.78 A
23		2099	NZ	LYS				9.552 -13.368	1.00 29.76 A
	ATOM			LYS			83.979		
	ATOM	2100	C				88.065	14.120 -16.576	1.00 21.13 A
	MOTA	2101	0	LYS			89.170	13.631 -16.362	1.00 21.11 A
	MOTA	2102	N	ALA			87.697	14.549 -17.780	1.00 21.55 A
30	MOTA	2103	CA	ALA			88.600	14.426 -18.922	1.00 22.23 A
	MOTA	2104	CB	ALA			87.802	14.368 -20.221	1.00 21.66 A
	ATOM	2105	C	ALA			89.604	15.569 -18.988	1.00 23.04 A
	MOTA	2106	0	ALA			90.518	15.541 -19.800	1.00 22.63 A
	MOTA	2107	N	HIS	Α	339	89.447	16.570 -18.131	1.00 23.26 A
35	MOTA	2108	CA	HIS	Α	339	90.362	17.705 -18.148	1.00 23.33 A
	ATOM	2109	CB	HIS	Α	339	90.017	18.680 -17.027	1.00 22.99 A
	MOTA	2110	CG	HIS	Α	339	90.696	20.004 -17.156	1.00 23.43 A
	MOTA	2111	CD2	HIS	Α	339	90.279	21.168 -17.710	1.00 24.32 A
	ATOM	2112	ND1	HIS	Α	339	91.993	20.219 -16.741	1.00 22.64 A
40	ATOM	2113		HIS			92.346	21.459 -17.036	1.00 24.03 A
	ATOM	2114		HIS			91.324	22.056 -17.626	1.00 23.65 A
	ATOM	2115	C	HIS			91.833	17.302 -18.046	1.00 24.36 A
	ATOM	2116	ō	HIS			92.186	16.376 -17.317	1.00 24.27 A
	ATOM	2117	N	PRO			92.713	17.999 -18.788	1.00 25.89 A
45	ATOM	2118	CD	PRO			92.394	19.050 -19.777	1.00 26.27 A
75	ATOM	2119	CA	PRO			94.151	17.714 -18.785	1.00 26.69 A
	ATOM	2120	CB	PRO			94.727	18.861 -19.613	1.00 26.46 A
	MOTA	2121	CG	PRO			93.654	19.090 -20.636	1.00 25.56 A
	MOTA	2122	C	PRO			94.772	17.629 -17.396	1.00 27.13 A
50	MOTA	2123	0	PRO			95.686	16.841 -17.167	1.00 28.89 A
	MOTA	2124	N	PHE			94.281	18.438 -16.466	1.00 26.76 A
	MOTA	2125	CA	PHE			94.815	18.417 -15.110	1.00 25.83 A
	MOTA	2126	CB	PHE			94.100	19.451 -14.239	1.00 24.58 A
	MOTA	2127	CG	PHE			94.628	19.527 -12.835	1.00 23.75 A
55	MOTA	2128		PHE			95.890	20.060 -12.578	1.00 24.62 A
	ATOM	2129	CD2	PHE	Α	341	93.867	19.066 -11.765	1.00 24.82 A
	ATOM	2130	CE1	PHE	Α	341	96.386	20.136 -11.273	1.00 23.48 A
	ATOM	2131	CE2	PHE	Α	341	94.352	19.136 -10.454	1.00 23.61 A
	ATOM	2132	CZ	PHE	Α	341	95.614	19.673 -10.209	1.00 23.80 A

	MOTA	2133	C	PHE	Α	341	94.684	17.039 -14.458	1.00 25.53 A
	ATOM	2134	0	PHE	Α	341	95.453	16.698 -13.572	1.00 25.60 A
	ATOM	2135	N	PHE	Α	342	93.718	16.248 -14.905	1.00 26.56 A
	ATOM	2136	CA	PHE	Α	342	93.486	14.928 -14.327	1.00 28.32 A
5	ATOM	2137	CB	PHE	Α	342	91.992	14.724 -14.095	1.00 25.63 A
	MOTA	2138	CG	PHE	А	342	91.374	15.731 -13.169	1.00 24.19 A
	ATOM	2139	CD1	PHE	А	342	91.830	15.868 -11.859	1.00 24.72 A
	ATOM	2140	CD2	PHE	А	342	90.285	16.492 -13.579	1.00 21.46 A
	ATOM	2141		PHE			91.200	16.744 -10.969	1.00 22.95 A
10	ATOM	2142	CE2	PHE			89.649	17.368 -12.699	1.00 19.82 A
	ATOM	2143	CZ	PHE			90.105	17.491 -11.393	1.00 20.87 A
	ATOM	2144	C	PHE			94.009	13.811 -15.217	1.00 31.08 A
	ATOM	2145	Ö	PHE			93.655	12.643 -15.047	1.00 32.72 A
	ATOM	2146	N	GLU			94.863	14.183 -16.159	1.00 32.72 A
15	ATOM	2147	CA	GLU			95.446	13.250 -17.114	1.00 36.10 A
15	ATOM	2148	CB	GLU			96.738	13.853 -17.676	1.00 38.76 A
	ATOM	2149	CG	GLU			96.842	13.883 -19.194	1.00 44.39 A
	ATOM	2150	CD	GLU			96.911	15.307 -19.750	1.00 48.43 A
20	ATOM	2151		GLU			97.665	16.143 -19.190	1.00 47.87 A
20	ATOM	2152		GLU			96.217	15.587 -20.755	1.00 49.34 A
	ATOM	2153	С	GLU		343	95.747	11.855 -16.552	1.00 35.54 A
	MOTA	2154	0	GLU			95.210	10.847 -17.019	1.00 33.70 A
	MOTA	2155	N	SER			96.604	11.810 -15.539	1.00 34.66 A
	MOTA	2156	CA	SER			97.024	10.545 -14.950	1.00 33.91 A
25	MOTA	2157	CB	SER			98.421	10.712 -14.360	1.00 33.13 A
	MOTA	2158	OG	SER			98.387	11.578 -13.242	1.00 30.32 A
	MOTA	2159	C	SER			96.116	9.927 -13.886	1.00 33.50 A
	MOTA	2160	0	SER			96.510	8.962 -13.234	1.00 32.98 A
	MOTA	2161	N	VAL			94.908	10.448 -13.713	1.00 31.80 A
30	MOTA	2162	CA	VAL			94.021	9.903 -12.689	1.00 31.70 A
	MOTA	2163	CB	VAL		345	93.039	10.981 -12.152	1.00 31.20 A
	ATOM	2164		VAL			92.153	10.375 -11.079	1.00 29.96 A
	MOTA	2165	CG2	VAL	Α	345	93.799	12.176 -11.601	1.00 27.23 A
	MOTA	2166	C	VAL	Α	345	93.175	8.707 -13.133	1.00 32.88 A
35	ATOM	2167	0	VAL	Α	345	92.597	8.712 -14.223	1.00 32.39 A
	ATOM	2168	N	THR	Α	346	93.109	7.688 -12.279	1.00 31.88 A
	ATOM	2169	CA	THR	Α	346	92.285	6.511 -12.539	1.00 32.94 A
	ATOM	2170	CB	THR	Α	346	93.007	5.209 -12.149	1.00 35.61 A
	ATOM	2171	OG1	THR	Α	346	94.137	5.012 -13.013	1.00 37.85 A
40	ATOM	2172	CG2	THR	Α	346	92.060	4.022 -12.267	1.00 32.32 A
	MOTA	2173	C	THR	Α	346	91.051	6.700 -11.658	1.00 33.08 A
	ATOM	2174	0	THR	Α	346	91.083	6.460 -10.448	1.00 34.21 A
	ATOM	2175	N	TRP	Α	347	89.964	7.142 -12.274	1.00 31.78 A
	ATOM	2176	CA	TRP	Α	347	88.741	7.427 -11.549	1.00 31.53 A
45	ATOM	2177	CB	TRP	Α	347	87.769	8.171 -12.463	1.00 28.28 A
	MOTA	2178	CG	TRP	А	347	88.303	9.476 -12.937	1.00 23.66 A
	ATOM	2179		TRP		347	88.263	10.722 -12.231	1.00 23.03 A
	ATOM	2180	CE2	TRP			88.927	11.678 -13.031	1.00 20.77 A
	ATOM	2181		TRP		347	87.731	11.121 -10.999	1.00 20.57 A
50	ATOM	2182		TRP		347	88.969	9.718 -14.102	1.00 21.92 A
	ATOM	2183		TRP		347	89.348	11.041 -14.168	1.00 22.23 A
	ATOM	2184	CZ2	TRP		347	89.074	13.008 -12.640	1.00 21.04 A
	ATOM	2185		TRP			87.876	12.444 -10.611	1.00 20.11 A
	ATOM	2186		TRP		347	88.544	13.372 -11.430	1.00 20.11 A
55	ATOM	2187	Cnz	TRP			88.014	6.267 -10.899	1.00 20.44 A
22	ATOM	2188	0	TRP		347	87.382	6.440 -9.854	1.00 34.19 A
	ATOM	2188	N	GLU		347	88.108	5.089 -11.502	1.00 34.97 A 1.00 35.77 A
	ATOM	2199	CA	GLU			87.405	3.913 -11.000	1.00 35.77 A
	MOTA	2191	CB	GLU	Α	348	87.600	2.740 -11.977	1.00 36.95 A

	ATOM	2192	CG	GLU A		88.990		-12.588	0.00 36.86 A	
	ATOM	2193	CD	GLU A	348	89.173	3.510	-13.812	0.00 36.91 A	
	ATOM	2194	OE1	GLU A	348	89.119	4.750	-13.677	0.00 36.92 A	
	MOTA	2195	OE2	GLU A	348	89.370	2.960	-14.916	0.00 36.92 A	
5	ATOM	2196	C	GLU A	348	87.668	3.435	-9.563	1.00 36.38 A	
	ATOM	2197	0	GLU A	348	86.773	2.866	-8.935	1.00 38.29 A	
	ATOM	2198	N	ASN A	349	88.857	3.669	-9.019	1.00 34.41 A	
	ATOM	2199	CA	ASN A	349	89.134	3.182	-7.668	1.00 33.02 A	
	ATOM	2200	CB	ASN A		89.848	1.844	-7.765	1.00 34.07 A	
10	ATOM	2201	CG	ASN A	349	91.220	1.978	-8.381	1.00 35.48 A	
	ATOM	2202		ASN A		91.409	2.742	-9.324	1.00 35.13 A	
	ATOM	2203		ASN A		92.188	1.235	-7.852	1.00 38.04 A	
	ATOM	2204	С	ASN A		89.970	4.116	-6.804	1.00 30.73 A	
	ATOM	2205	ō	ASN A		90.878	3.672	-6.106	1.00 30.66 A	
15	ATOM	2206	N	LEU A		89.662	5.403	-6.850	1.00 28.42 A	
	ATOM	2207	CA	LEU A		90.390	6.397	-6.072	1.00 27.13 A	
	ATOM	2208	CB	LEU A		89.655	7.737	-6.128	1.00 25.19 A	
	ATOM	2209	CG	LEU A		89.803	8.543	-7.418	1.00 25.13 A	
	ATOM	2210		LEU A		88.841	9.732	-7.428	1.00 26.30 A	
20	ATOM	2211		LEU A		91.242	9.014	-7.521	1.00 20.30 A	
20	ATOM	2212	C	LEU A		90.581	5.999	-4.614	1.00 26.30 A	
	ATOM	2213	0	LEU A		91.645	6.201	-4.036	1.00 26.73 A	
	ATOM	2214	N	HIS A		89.547	5.424	-4.024	1.00 20.75 A	
	ATOM	2215	CA	HIS A		89.593	5.044	-2.622	1.00 27.16 A	
25				HIS A					1.00 28.60 A	
25	ATOM	2216	CB			88.184	4.748	-2.124		
	ATOM	2217	CG	HIS A		88.111	4.503	-0.653	1.00 30.99 A	
	ATOM	2218				88.324	5.329	0.399	1.00 31.86 A	
	MOTA	2219		HIS A		87.790	3.275	-0.118	1.00 29.43 A	
20	ATOM	2220		HIS A		87.804	3.356	1.202	1.00 31.81 A	
30	ATOM	2221	NE2			88.125	4.592	1.541	1.00 32.90 A	
	ATOM	2222	С	HIS A		90.509	3.873	-2.298	1.00 28.99 A	
	ATOM	2223	0	HIS A		90.875	3.677	-1.141	1.00 28.53 A	
	MOTA	2224	N	GLN A		90.865	3.088	-3.307	1.00 30.57 A	
	MOTA	2225	CA	GLN A		91.764	1.959	-3.095	1.00 33.42 A	
35	ATOM	2226	CB	GLN A		91.563	0.880	-4.162	1.00 35.01 A	
	ATOM	2227	CG	GLN A		90.696	-0.289	-3.737	1.00 37.07 A	
	MOTA	2228	CD	GLN A		89.275	0.123	-3.474	1.00 39.83 A	
	MOTA	2229		GLN A		88.676	0.856	-4.267	1.00 41.90 A	
	MOTA	2230	NE2			88.712	-0.351	-2.365	1.00 39.86 A	
40	MOTA	2231	С	GLN A		93.197	2.457	-3.173	1.00 33.85 A	
	MOTA	2232	0	GLN A		94.126	1.782	-2.734	1.00 35.32 A	
	MOTA	2233	N	GLN A		93.368	3.647	-3.734	1.00 32.53 A	
	MOTA	2234	CA	GLN A		94.693	4.216	-3.886	1.00 32.78 A	
	MOTA	2235	CB	GLN A		94.666	5.298	-4.965	1.00 32.07 A	
45	MOTA	2236	CG	GLN A		94.373	4.739	-6.345	1.00 31.94 A	
	MOTA	2237	CD	GLN A		94.206	5.819	-7.382	1.00 32.50 A	
	MOTA	2238		GLN A		95.008	6.749	-7.452	1.00 35.33 A	
	MOTA	2239	NE2			93.167	5.701	-8.204	1.00 31.02 A	
	MOTA	2240	C	GLN A	353	95.246	4.779	-2.588	1.00 33.27 A	
50	MOTA	2241	0	GLN A	353	94.494	5.209	-1.717	1.00 32.38 A	
	MOTA	2242	N	THR A	354	96.570	4.746	-2.462	1.00 33.29 A	
	ATOM	2243	CA	THR A	354	97.239	5.267	-1.280	1.00 34.35 A	
	ATOM	2244	CB	THR A	354	98.615	4.601	-1.069	1.00 35.88 A	
	ATOM	2245	OG1	THR A	354	98.430	3.232	-0.690	1.00 36.70 A	
55	ATOM	2246	CG2	THR A	354	99.403	5.325	0.027	1.00 36.08 A	
	ATOM	2247	C	THR A	354	97.440	6.760	-1.478	1.00 33.06 A	
	ATOM	2248	0	THR A	354	98.120	7.181	-2.403	1.00 31.33 A	
	ATOM	2249	N	PRO A	355	96.844	7.581	-0.604	1.00 33.40 A	
	ATOM	2250	CD	PRO A	355	96.000	7.220	0.544	1.00 31.90 A	

	MOTA	2251	CA	PRO	Α	355	96.974	9.035	-0.710	1.00 34.90 A
	MOTA	2252	CB	PRO	Α	355	96.156	9.543	0.475	1.00 33.68 A
	MOTA	2253	CG	PRO	Α	355	95.160	8.452	0.698	1.00 33.37 A
	MOTA	2254	C	PRO	Α	355	98.428	9.475	-0.623	1.00 36.27 A
5	ATOM	2255	0	PRO	Α	355	99.196	8.960	0.191	1.00 35.70 A
	MOTA	2256	N	PRO	А	356	98.824	10.433	-1.464	1.00 37.66 A
	MOTA	2257	CD	PRO	А	356	98.010	11.198	-2.423	1.00 38.22 A
	ATOM	2258	CA	PRO		356	100.205	10.916	-1.441	1.00 39.93 A
	ATOM	2259	CB	PRO		356	100.227	11.944	-2.570	1.00 38.83 A
10	ATOM	2260	CG	PRO		356	98.818	12.466	-2.580	1.00 38.26 A
	ATOM	2261	C	PRO		356	100.532	11.534	-0.085	1.00 41.87 A
	ATOM	2262	o	PRO		356	99.696	12.209	0.506	1.00 40.91 A
	ATOM	2263	N	ALA			101.741	11.286	0.409	1.00 46.23 A
	ATOM	2264	CA	ALA		357	102.160	11.837	1.691	1.00 40.25 A
15	ATOM	2265	CB	ALA		357	103.587	11.410	2.001	1.00 31.16 A
13	ATOM	2266	C	ALA		357	102.077	13.354	1.589	1.00 49.78 A
	ATOM	2267	0	ALA		357	102.591	13.942	0.637	1.00 55.14 A
	MOTA	2268	N	LEU		358	101.419	13.985	2.559	1.00 58.59 A
20	MOTA	2269	CA	LEU		358	101.276	15.437	2.552	1.00 62.92 A
20	MOTA	2270	CB	LEU		358	100.107	15.866	3.441	1.00 62.51 A
	MOTA	2271	CG	LEU		358	98.732	15.752	2.783	1.00 63.05 A
	MOTA	2272		LEU		358	97.657	16.251	3.737	1.00 63.34 A
	ATOM	2273		LEU		358	98.721	16.570	1.494	1.00 62.56 A
	MOTA	2274	C	LEU		358	102.536	16.173	2.984	1.00 65.81 A
25	MOTA	2275	0	LEU		358	102.675	16.559	4.148	1.00 66.45 A
	MOTA	2276	N	THR		359	103.441	16.368	2.025	1.00 69.31 A
	MOTA	2277	CA	THR		359	104.715	17.057	2.236	1.00 72.25 A
	MOTA	2278	CB	THR		359	104.519	18.594	2.271	1.00 73.17 A
	MOTA	2279	og1	THR	Α	359	103.564	18.937	3.284	1.00 75.38 A
30	ATOM	2280	CG2	THR	Α	359	104.030	19.101	0.916	1.00 72.93 A
	ATOM	2281	C	THR	Α	359	105.468	16.627	3.497	1.00 73.76 A
	MOTA	2282	0	THR	Α	359	105.011	15.683	4.180	1.00 74.61 A
	MOTA	2283	OXT	THR	Α	359	106.523	17.237	3.780	1.00 75.50 A
	ATOM	2284	OH2	TIP	S	1	82.965	32.402	-3.946	1.00 13.32 S
35	ATOM	2285	OH2	TIP	s	2	91.556	13.784	-17.557	1.00 22.11 S
	ATOM	2286	OH2	TIP	s	3	87.391	33.155	-1.722	1.00 22.84 S
	MOTA	2287	OH2	TIP	s	4	69.033	3.499	13.879	1.00 22.91 S
	MOTA	2288	OH2	TIP	s	5	81.088	19.368	-18.406	1.00 24.13 S
	ATOM	2289	OH2	TIP	s	6	75.641	16.130	8.209	1.00 26.44 S
40	ATOM	2290	OH2	TIP	s	7	74.760	20.961	3.347	1.00 27.74 S
	ATOM	2291	OH2	TIP	s	8	75.152	6.784	5.545	1.00 22.53 S
	ATOM	2292	OH2	TIP	s	9	77.282		-17.666	1.00 35.96 S
	ATOM	2293	OH2	TIP	S	10	81.785	8.968	-8.072	1.00 25.44 S
	ATOM	2294		TIP	s	11	78.609	24.424	-2.074	1.00 22.05 S
45	ATOM	2295	OH2	TIP	S	12	94.883	8.256	-9.981	1.00 37.17 S
	ATOM	2296	OH2	TIP	s	13	73.164	38.970	-1.072	1.00 35.95 S
	ATOM	2297	OH2	TIP	S	14	78.806	27.556	-3.116	1.00 39.27 S
	ATOM	2298		TIP	S	15	89.050	8.041	10.604	1.00 33.27 S
	ATOM	2299		TIP	S	16	73.265	40.376	-3.301	1.00 25.40 S
50	ATOM	2300			S	18	84.081	33.371	4.243	1.00 20.54 S
30		2300	OH2	TIP			78.571	-0.530	16.531	
	MOTA				S	19				
	ATOM	2302	OH2	TIP	S	21	70.088	3.703	17.559	1.00 28.94 S
	MOTA	2303		TIP	S	22	79.212		-18.791	1.00 26.94 S
	MOTA	2304		TIP	S	23	91.672		-16.153	1.00 30.26 S
55	MOTA	2305	OH2	TIP	S	25	104.173	17.689	-7.204	1.00 31.65 S
	MOTA	2306	OH2	TIP	S	27	87.578		-20.604	1.00 25.98 S
	MOTA	2307	OH2	TIP	S	28	82.272		-16.021	1.00 27.40 S
	MOTA	2308	OH2		S	29	100.496	13.074	-9.812	1.00 37.92 S
	MOTA	2309	OH2	TIP	S	30	65.147	10.515	28.440	1.00 40.03 S

	MOTA	2310	OH2	TIP	S	31	90.721	38.800	-4.631	1.00	42.09 S	
	MOTA	2311	OH2	TIP	S	32	83.367	23.841	15.654	1.00	36.15 S	i
	MOTA	2312	OH2	TIP	S	33	87.754	11.897	23.760	1.00	26.76 S	
	MOTA	2313	OH2	TIP	S	34	77.755	13.485	-15.395	1.00	31.85 S	5
5	ATOM	2314	OH2	TIP	s	35	79.767	43.115	5.371	1.00	35.26 S	5
	ATOM	2315	OH2	TIP	s	37	80.173	32.998	6.198	1.00	40.03 S	5
	ATOM	2316	OH2	TIP	S	40	85.958	19.110	24.502	1.00	24.42 S	5
	ATOM	2317	OH2	TIP	s	42	77.719	-0.391	23.732		39.71 S	
	ATOM	2318	OH2	TIP	s	44	92.563	36.428	-5.574		35.43 S	
10	ATOM	2319	OH2	TIP	s	45	90.942	34.092	3.570		43.64 S	
	ATOM	2320	OH2	TIP	S	46	74.357		-13.849		33.31 S	
	ATOM	2321	OH2	TIP	S	47	90.220	14.449	16.172		34.34 S	
	ATOM	2322	OH2		S	48	77.876		-13.863		23.53 S	
	ATOM	2323	OH2	TIP	S	50	76.289		-11.572		37.74 S	
15	ATOM	2323	OH2	TIP	S	51	76.619	2.787	-2.969		35.95 S	
13	ATOM	2324	OH2	TIP		52	65.118	19.629	24.370			
					S							
	ATOM	2326	OH2	TIP	S	53	99.690		-13.046		48.21 S	
	MOTA	2327	OH2	TIP	S	54	88.376	36.865	3.454		38.54 S	
	MOTA	2328	OH2	TIP	S	57	91.236	10.819	18.279		40.76 S	
20	MOTA	2329	OH2	TIP	S	59	100.017		-14.622		41.65 S	
	MOTA	2330	OH2	TIP	S	63	87.188	25.521	11.438		41.53 S	
	MOTA	2331	OH2	TIP	S	65	90.264	19.625	12.286		24.22 S	
	ATOM	2332	OH2	TIP	S	66	83.805		-18.365		37.50 S	
	MOTA	2333	OH2	TIP	S	68	78.394	7.378	2.855		23.47 S	
25	ATOM	2334	OH2	TIP	S	74	85.541		-18.436		37.35 S	
	MOTA	2335	OH2	TIP	S	76	98.981	8.707	2.808		47.34 S	
	MOTA	2336	OH2	TIP	S	78	87.802	19.118	22.522	1.00	39.99 S	
	MOTA	2337	OH2	TIP	S	80	92.438	3.105	2.517	1.00	37.27 S	
	MOTA	2338	OH2	TIP	s	81	75.580	-0.821	22.186	1.00	36.41 S	
30	ATOM	2339	OH2	TIP	s	82	60.506	24.278	21.938	1.00	31.55 S	
	MOTA	2340	OH2	TIP	S	83	92.298	22.520	-21.183	1.00	42.32 S	
	MOTA	2341	OH2	TIP	S	84	74.351	4.211	-3.464	1.00	32.53 S	
	ATOM	2342	OH2	TIP	S	85	76.502	25.963	-21.839	1.00	41.89 S	
	ATOM	2343	OH2	TIP	S	86	97.965	13.142	9.216	1.00	41.76 S	
35	ATOM	2344	OH2	TIP	s	87	78.657	4.418	3.361	1.00	35.63 S	
	ATOM	2345	OH2	TIP	s	88	93.633	28.572	3.429	1.00	34.30 S	
	MOTA	2346	OH2	TIP	S	89	104.691	20.306	-7.235	1.00	32.75 S	
	MOTA	2347	OH2	TIP	S	91	98.360	16.754	-15.558	1.00	37.92 S	
	ATOM	2348	OH2	TIP	s	92	88.175	32.723	-14.088	1.00	38.91 S	
40	ATOM	2349	OH2	TIP	s	93	96.974		-17.613		34.47 S	
	ATOM	2350	OH2	TIP	s	94	85.585	22.346	15.199		41.12 S	
	ATOM	2351	OH2	TIP	S	100	80.948	-0.010	7.892		12.04 S	
	ATOM	2352	OH2	TIP	s	101	76.653	29.202	-3.527		22.10 S	
	ATOM	2353			s	102	74.980	8.979	-7.975		21.17 S	
45	ATOM	2354	OH2	TIP	S	103	88.843	28.393	3.994		30.94 S	
	ATOM	2355	OH2	TIP	S	105	76.862	8.067	28.490		20.20 S	
	ATOM	2356	OH2	TIP	S	106	66.435	30.702	8.817		35.87 S	
	ATOM	2357	OH2	TIP	S	100	67.384	7.757	8.860		39.38 S	
	ATOM	2358	OH2	TIP	S	110	66.852	4.666	22.301		32.75 S	
50	ATOM	2359		TIP		111	72.391	2.229	-3.501		51.07 S	
50	ATOM		OH2	TIP		116	80.209	7.061	-7.886			
		2360			S							
	ATOM	2361	OH2	TIP	S	121	74.466		-12.357		45.36 S	
	MOTA	2362	OH2	TIP	S	122	79.225	28.627	0.179		30.68 S	
	MOTA	2363	OH2	TIP	S	124	59.090	22.126	22.498		35.94 S	
55	MOTA	2364	OH2	TIP	S	126	73.715		-13.973		44.35 S	
	MOTA	2365	OH2	TIP	S	127	105.619		-11.256		43.80 S	
	MOTA	2366	OH2	TIP	S	128	86.658		-16.090		39.40 S	
	MOTA	2367	OH2	TIP	S	129	70.750		-10.875		45.74 S	
	MOTA	2368	OH2	TIP	S	136	77.820	12.663	6.090	1.00	47.18 S	į

	MOTA	2369		TIP			90.942		-13.582	1.00 48.16 S
	ATOM	2370	OH2	TIP	s	146	67.351	6.830	24.075	1.00 36.66 S
	MOTA	2371	OH2	TIP	S	148	98.067	12.182	-7.216	1.00 38.66 S
	ATOM	2372	OH2	TIP	S	156	75.211	13.809	-20.582	1.00 45.56 S
5	ATOM	2373	OH2	TIP	s	158	72.261	20.575	12.175	1.00 51.45 S
	MOTA	2374	OH2	TIP	s	166	77.289	42.685	7.086	1.00 42.23 S
	ATOM	2375	OH2	TIP	S	174	65.330	6.552	20.003	1.00 42.22 S
	ATOM	2376	OH2	TIP		176	88.027		-20.665	1.00 35.09 S
	ATOM	2377		TIP		178	99.488		-16.497	1.00 44.21 S
10	ATOM	2378	OH2		s	182	93.851		-20.448	1.00 50.19 S
	ATOM	2379	OH2			192	83.811	26.388	9.460	1.00 39.52 S
	ATOM	2380	OH2	TIP		193	91.704	42.080	2.405	1.00 39.52 S
	ATOM	2381		GLC		1	82.624	0.887	12.473	1.00 47.94 G
		2382				1	82.240	2.160	13.000	
1.5	ATOM				G					
15	MOTA	2383		GLC		1	83.237	3.235	12.553	1.00 46.87 G
	MOTA	2384		GLC		1	84.544	2.903	13.022	1.00 46.62 G
	MOTA	2385		GLC		1	82.817	4.591	13.117	1.00 45.80 G
	MOTA	2386			G	1	83.746	5.589	12.703	1.00 43.50 G
	MOTA	2387		GLC		5	86.722	-2.593	0.107	1.00 39.62 G
20	MOTA	2388		GLC		5	86.245	-1.364	-0.429	1.00 44.37 G
	MOTA	2389		GLC		5	86.764	-0.193	0.394	1.00 44.36 G
	MOTA	2390	014	GLC	G	5	86.355	-0.326	1.761	1.00 47.64 G
	ATOM	2391	C15	GLC	G	5	86.231	1.132	-0.195	1.00 45.11 G
	MOTA	2392	016	GLC	G	5	86.666	1.310	-1.557	1.00 42.61 G
25	ATOM	2393	012	GLC	G	8	87.512	4.414	-5.278	1.00 38.37 G
	ATOM	2394	C11	GLC	G	8	86.362	5.220	-5.023	1.00 34.16 G
	ATOM	2395	C13	GLC	G	8	85.750	5.654	-6.351	1.00 35.54 G
	ATOM	2396	014	GLC	G	8	86.717	6.392	-7.111	1.00 37.03 G
	ATOM	2397	C15	GLC	G	8	84.521	6.523	-6.082	1.00 35.46 G
30	ATOM	2398		GLC	G	8	83.948	6.931	-7.319	1.00 33.79 G
	ATOM	2399	C34	STO		1	82.178	19.404	9.614	1.00 23.98 L
	ATOM	2400		STO		ī	83.091	19.645	10.691	1.00 24.40 L
	ATOM	2401		STO		ī	82.557	20.621	11.610	1.00 19.84 L
	ATOM	2402		STO		1	83.748	21.455	12.055	1.00 20.35 L
35	ATOM	2403	N31			1	84.251	22.242	10.916	1.00 20.55 L
33	ATOM	2403	C32	STO		1	83.716	23.544	10.481	1.00 22.36 L
						1				
	ATOM	2405	C27	STO			84.847	20.523	12.559	1.00 19.37 L
	ATOM	2406	C28	STO		1	84.278	19.595	13.658	1.00 18.70 L
40	ATOM	2407	029	STO		1	82.889	19.845	13.980	1.00 20.08 L
40	MOTA	2408	C24	STO		1	81.939	19.930	12.872	1.00 21.85 L
	MOTA	2409	C35	STO		1	80.791	20.824	13.403	1.00 20.12 L
	MOTA	2410	N6	STO		1	81.456	18.689	12.528	1.00 19.30 L
	MOTA	2411	C5	STO		1	80.172	18.450	12.023	1.00 16.04 L
	MOTA	2412	C4	STO		1	79.039	19.219	11.690	1.00 14.17 L
45	ATOM	2413	C3	STO	L	1	77.901	18.569	11.148	1.00 14.32 L
	MOTA	2414	C2	STO	L	1	77.899	17.158	10.946	1.00 14.05 L
	ATOM	2415	C1	STO	L	1	79.035	16.386	11.282	1.00 13.54 L
	ATOM	2416	C23	STO	L	1	80.154	17.053	11.812	1.00 16.42 L
	MOTA	2417	C22	STO	L	1	81.361	16.522	12.164	1.00 17.74 L
50	ATOM	2418	C7	STO	L	1	82.162	17.525	12.606	1.00 18.84 L
	ATOM	2419	C8	STO	L	1	83.501	17.279	12.972	1.00 18.69 L
	ATOM	2420	N9	STO		1	84.462	18.150	13.376	1.00 19.59 L
	ATOM	2421		STO		1	85.663	17.477	13.561	1.00 19.11 L
	ATOM	2422	C11		L	1	86.968	17.838	13.942	1.00 16.81 L
55	ATOM	2423	C12	STO		1	87.961	16.831	14.007	1.00 20.66 L
	ATOM	2424	C13	STO		1	87.645	15.476	13.689	1.00 20.30 L
	ATOM	2425	C14	STO		1	86.329	15.117	13.306	1.00 20.30 L
	ATOM	2425	C15	STO		1	85.364	16.127	13.248	1.00 19.86 L
				STO		1				1.00 10.74 L
	ATOM	2427	CTP	STU	ь	1	84.049	16.022	12.899	1.00 19.21 L

	MOTA	2428		STO		1	83.217	14.936		1.00 18.26 L
	MOTA	2429	C21			1	81.934	15.217		1.00 17.21 L
	MOTA	2430	C20			1	81.325	14.098		1.00 17.68 L
	MOTA	2431	N19			1	82.281	13.080		1.00 13.64 L
5	MOTA	2432	C18	STO		1	83.457	13.603		1.00 16.89 L
	MOTA	2433		STO		1	84.493	12.981		1.00 15.41 L
	MOTA	2434	S	SO4		1	64.914	7.877		1.00 82.11 I
	MOTA	2435	01	SO4		1	63.624	8.415		1.00 82.68 I
	MOTA	2436	02	SO4		1	65.841	8.992		1.00 82.73 I
10	MOTA	2437	03	SO4		1	65.479	7.010		1.00 83.33 I
	MOTA	2438	04	SO4		1	64.709	7.088		1.00 82.04 I
	MOTA	2439	S	SO4		2	68.379	-7.029		1.00112.82 I
	MOTA	2440	01	SO4		2	66.992	-6.526		1.00112.60 I
	MOTA	2441	02	SO4		2	68.850	-7.226		1.00112.21 I
15	MOTA	2442	03	SO4		2	68.426	-8.312		1.00112.24 I
	MOTA	2443	04	SO4		2	69.249	-6.051		1.00112.72 I
	MOTA	2444	S	SO4		3	84.927	-1.874		1.00 79.99 I
	MOTA	2445	01	SO4	I	3	84.408	-1.334	13.568	1.00 79.90 I
	MOTA	2446	02	SO4	I	3	84.442	-1.050	11.178	1.00 80.43 I
20	MOTA	2447	03	SO4	I	3	84.453	-3.263		1.00 79.92 I
	MOTA	2448	04	SO4		3	86.402	-1.845		1.00 80.52 I
	MOTA	2449	S	SO4	I	4	80.577	9.632	30.033	1.00 98.23 I
	MOTA	2450	01	SO4	I	4	79.725	9.060	28.972	1.00 96.88 I
	MOTA	2451	02	SO4	I	4	82.000	9.461	29.683	1.00 97.80 I
25	MOTA	2452	03	SO4	I	4	80.304	8.944	31.309	1.00 98.08 I
	MOTA	2453	04	SO4	I	4	80.281	11.069	30.178	1.00 98.08 I
	MOTA	2454	S	SO4	I	5	89.310	6.131	25.915	1.00110.86 I
	MOTA	2455	01	SO4	I	5	89.025	6.456	27.331	1.00110.48 I
	MOTA	2456	02	SO4	I	5	88.042	6.095	25.151	1.00110.12 I
30	MOTA	2457	03	SO4	I	5	89.970	4.810	25.844	1.00110.72 I
	MOTA	2458	04	SO4	I	5	90.205	7.155	25.330	1.00110.02 I
	MOTA	2459	02	PO4	Ρ	100	64.527	26.252	2.299	1.00 88.98 P
	MOTA	2460	03	PO4	Ρ	100	66.482	25.155	1.367	1.00 88.39 P
	MOTA	2461	04	PO4	P	100	66.688	26.504	3.376	1.00 87.87 P
35	MOTA	2462	01	PO4	Ρ	100	66.264	27.565	1.240	1.00 88.80 P
	MOTA	2463	P	PO4	Ρ	100	65.992	26.368	2.070	1.00 88.61 P
	MOTA	2464	CB	LEU		145	73.932	8.398	8.961	0.50 21.29 AC2
	MOTA	2465	CG	LEU		145	72.901	8.606	10.076	0.50 21.65 AC2
	MOTA	2466	CD1	LEU		145	71.904	9.671	9.655	0.50 21.60 AC2
40	MOTA	2467	CD2	LEU		145	72.195	7.298	10.388	0.50 19.61 AC2
	MOTA	2468	CB	ASN		214	88.968	8.625	7.173	0.50 22.34 AC2
	MOTA	2469	CG	ASN		214	89.705	8.084	5.975	0.50 22.01 AC2
	MOTA	2470	OD1	ASN		214	89.240	7.153	5.320	0.50 22.82 AC2
	MOTA	2471	ND2	ASN		214	90.859	8.660	5.678	0.50 22.69 AC2
45	MOTA	2472	CB	ASP		216	93.187	5.546	5.379	0.50 25.98 AC2
	MOTA	2473	CG	ASP		216	91.789	5.828		0.50 27.09 AC2
	ATOM	2474	OD1	ASP		216	91.587	6.896	4.290	0.50 28.49 AC2
	MOTA	2475		ASP		216	90.896	4.982		0.50 28.20 AC2
	END									

Example 8: Co-ordinates for PDK1 fragment co-crystallised with UCN-

01 REMARK coordinates from restrained individual B-factor refinement REMARK refinement resolution: 25.0 - 2.50 A REMARK starting r= 0.1919 free r= 0.2582 r= 0.1894 free r= 0.2567 REMARK final REMARK B rmsd for bonded mainchain atoms= 1.412 target= 1.5 REMARK B rmsd for bonded sidechain atoms= 2.205 target= 2.0 REMARK B rmsd for angle mainchain atoms= 2.401 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.256 target= 2.5 REMARK rweight= 0.1000 (with wa= 3.1611) REMARK target= mlf steps= 30 REMARK sg= P3(2)21 a= 123.387 b= 123.387 c= 47.115 alpha= 90 beta= 90 gamma= 120 REMARK parameter file 1 : /ddl/david/refinement/MY CNS/prot.par REMARK parameter file 2 : /ddl/david/refinement/MY_CNS/ucn01.par REMARK parameter file 3 : CNS_TOPPAR:water_rep.param REMARK parameter file 4 : CNS_TOPPAR:ion.param REMARK parameter file 5 : /dd1/david/refinement/MY CNS/glycerol.par REMARK molecular structure file: ../generate/generate.mtf REMARK input coordinates: ../minimize/minimize.pdb REMARK reflection file= ../../../data/cns.hkl REMARK nos= none REMARK B-correction resolution: 6.0 - 2.50 REMARK initial B-factor correction applied to fobs : REMARK B11= -4.722 B22= -4.722 B33= 9.444 REMARK B12= -3.572 B13= 0.000 B23= 0.000 -0.193 REMARK B-factor correction applied to coordinate array B: 30 REMARK bulk solvent: density level= 0.3837 e/A^3, B-factor= 40.9071 A^2 REMARK reflections with |Fobs|/sigma F < 0.0 rejected REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected REMARK theoretical total number of refl. in resol. range: 14485 (100.0 %) REMARK number of unobserved reflections (no entry or |F|=0): 101 (0.7 %) REMARK number of reflections rejected: 0 (0.0 %) REMARK total number of reflections used: 14384 (99.3 %) REMARK number of reflections in working set: 13795 (95.2 %) REMARK number of reflections in test set: 589 (4.1 %) CRYST1 123.387 123.387 47.115 90.00 90.00 120.00 P 32 2 1 REMARK FILENAME="bindividual.pdb" REMARK DATE: 25-Mar-2003 17:21:21 created by user: david REMARK VERSION: 1.0 1 CB ALA A 73 67.051 -3.293 12.591 1.00 59.77 A ATOM ATOM 2 C ALA A 73 67.941 -4.753 14.416 1.00 61.14 A 3 O ALA A 73 67.184 -5.270 15.240 1.00 61.61 A ATOM ATOM 4 N ALA A 73 66.523 -5.729 12.643 1.00 58.89 A ATOM 5 CA ALA A 73 67.564 -4.697 12.943 1.00 60.69 A ATOM 6 N PRO A 74 69.130 -4.241 14.770 1.00 61.63 A ATOM 7 CD PRO A 74 70.264 -3.830 13.918 1.00 61.72 A ATOM 8 CA PRO A 74 69.514 -4.278 16.187 1.00 61.34 A ATOM 9 CB PRO A 74 70.918 -3.663 16.181 1.00 61.79 A 71.458 -4.072 14.818 1.00 61.47 A 68.523 -3.481 17.047 1.00 60.16 A 67.625 -2.817 16.519 1.00 60.77 A

10 CG PRO A 74

11 C PRO A 74

12 O PRO A 74

ATOM

ATOM ATOM

	ATOM	13	N	ALA	A	75	68.680	-3.562	18.368	1.00 58.13 A
	MOTA	14	CA	ALA	A	75	67.815	-2.828	19.292	1.00 54.74 A
	ATOM	15	CB	ALA	Α	75	68.048	-3.309	20.731	1.00 54.90 A
	ATOM	16	С	ALA		75	68.175	-1.349	19.177	1.00 51.85 A
5	ATOM	17	ō	ALA		75	69.313	-1.005	18.851	1.00 52.46 A
-	ATOM	18	N	LYS		76	67.215	-0.473	19.427	1.00 46.96 A
	ATOM	19	CA	LYS		76	67.507	0.947	19.354	1.00 43.72 A
	ATOM	20	CB	LYS		76	66.270	1.756	19.744	1.00 42.81 A
	MOTA	21	CG	LYS		76	66.177	3.116	19.087	1.00 41.81 A
10	MOTA	22	CD	LYS	A	76	65.926	2.983	17.590	1.00 40.56 A
	MOTA	23	CE	LYS	A	76	65.691	4.343	16.943	1.00 42.58 A
	ATOM	24	NZ	LYS	A	76	65.362	4.231	15.495	1.00 42.73 A
	ATOM	25	C	LYS	A	76	68.639	1.218	20.351	1.00 41.25 A
	ATOM	26	0	LYS		76	68.599	0.741	21.488	1.00 41.68 A
15	ATOM	27	N		A	77	69.655	1.960	19.936	1.00 37.68 A
	ATOM	28	CA	LYS		77	70.748	2.255	20.849	1.00 35.10 A
		29				77		2.619	20.074	1.00 34.13 A
	ATOM		CB	LYS			72.016			
	MOTA	30	CG	LYS		77	72.427	1.570	19.053	1.00 32.68 A
	MOTA	31	CD		A	77	73.927	1.537	18.858	1.00 33.90 A
20	MOTA	32	CE	LYS		77	74.366	0.471	17.849	1.00 31.40 A
	MOTA	33	NZ	LYS	A	77	73.796	-0.863	18.164	1.00 34.76 A
	MOTA	34	C	LYS	A	77	70.313	3.408	21.743	1.00 34.79 A
	ATOM	35	0	LYS	A	77	69.319	4.077	21.458	1.00 34.20 A
	ATOM	36	N	ARG	А	78	71.023	3.626	22.845	1.00 34.88 A
25	ATOM	37	CA	ARG		78	70.687	4.723	23.759	1.00 34.62 A
	ATOM	38	CB	ARG		78	69.694	4.247	24.839	1.00 38.43 A
	ATOM	39	CG	ARG		78	70.027	2.884	25.353	1.00 42.71 A
	ATOM	40	CD	ARG		78	69.355	2.424	26.625	1.00 42.71 A
	MOTA	41	NE	ARG		78	70.365	1.702	27.412	1.00 56.10 A
30	ATOM	42	CZ	ARG		78	70.428	0.355	27.518	1.00 57.88 A
	MOTA	43		ARG		78	69.519	-0.397	26.838	1.00 58.45 A
	MOTA	44	NH2	ARG	A	78	71.335	-0.195	28.369	1.00 59.23 A
	MOTA	45	C	ARG	A	78	71.967	5.330	24.382	1.00 32.26 A
	ATOM	46	0	ARG	A	78	73.066	4.777	24.278	1.00 31.42 A
35	ATOM	47	N	PRO	А	79	71.844	6.509	24.997	1.00 30.46 A
	ATOM	48	CD	PRO		79	70.616	7.284	25.232	1.00 28.96 A
	ATOM	49	CA	PRO		79	72,997	7.172	25,609	1.00 30.38 A
	ATOM	50	CB	PRO		79	72.350	8.303	26.405	1.00 28.86 A
	ATOM	51	CG	PRO		79	71.169	8.642	25.568	1.00 27.83 A
40						79				
40	ATOM	52	С	PRO			73.889	6.287	26.468	1.00 29.47 A
	MOTA	53	0	PRO		79	75.108	6.377	26.391	1.00 29.57 A
	MOTA	54	N	GLU		80	73.268	5.435	27.279	1.00 29.77 A
	MOTA	55	CA	GLU		80	73.975	4.533	28.179	1.00 29.55 A
	MOTA	56	CB	GLU	A	80	72.980	3.768	29.043	1.00 32.88 A
45	MOTA	57	CG	GLU	A	80	71.996	4.643	29.798	1.00 40.36 A
	ATOM	58	CD	GLU	A	80	71.014	5.367	28.879	1.00 44.21 A
	MOTA	59	OE1	GLU	А	80	70.422	4.700	28.000	1.00 46.94 A
	ATOM	60		GLU		80	70.828	6.598	29.038	1.00 45.47 A
	ATOM	61	c	GLU		80	74.872	3.524	27.479	1.00 28.32 A
50	ATOM	62	o	GLU		80	75.709	2.894	28.126	1.00 28.20 A
50			N			81		3.342		1.00 26.28 A
	MOTA	63		ASP			74.698		26.168	
	MOTA	64	CA	ASP		81	75.528	2.384	25.441	1.00 23.59 A
	MOTA	65	CB	ASP		81	74.834	1.888	24.184	1.00 25.08 A
	MOTA	66	CG	ASP		81	73.510	1.225	24.477	1.00 28.14 A
55	MOTA	67		ASP		81	73.369	0.625	25.578	1.00 29.12 A
	MOTA	68		ASP		81	72.617	1.294	23.601	1.00 28.33 A
	MOTA	69	C		Α	81	76.856	2.967	25.046	1.00 23.24 A
	MOTA	70	0	ASP	Α	81	77.716	2.257	24.519	1.00 24.29 A
	ATOM	71	N	PHE	Α	82	77.036	4.259	25.309	1.00 21.34 A

	ATOM	72	CA	PHE		82	78.272	4.930	24.946	1.00 20.86 A
	MOTA	73	CB	PHE	А	82	77.992	6.029	23.929	1.00 18.34 A
	MOTA	74	CG	PHE		82	77.355	5.536	22.683	1.00 19.18 A
	MOTA	75	CD1	PHE	Α	82	78.138	5.099	21.610	1.00 19.28 A
5	ATOM	76	CD2	PHE	Α	82	75.974	5.462	22.588	1.00 17.82 A
	MOTA	77	CE1	PHE	Α	82	77.551	4.597	20.461	1.00 17.94 A
	ATOM	78	CE2	PHE	A	82	75.371	4.961	21.449	1.00 19.08 A
	ATOM	79	CZ	PHE	A	82	76.164	4.525	20.376	1.00 20.45 A
	ATOM	80	С	PHE	A	82	78.982	5.555	26.105	1.00 21.71 A
10	ATOM	81	0	PHE	A	82	78.418	5.739	27.173	1.00 24.82 A
	ATOM	82	N	LYS	А	83	80.244	5.865	25.869	1.00 21.83 A
	ATOM	83	CA	LYS		83	81.077	6.555	26.823	1.00 22.27 A
	ATOM	84	CB	LYS		83	82.327	5.750	27.148	1.00 24.03 A
	ATOM	85	CG	LYS		83	83.074	6.320	28.340	1.00 30.99 A
15	ATOM	86	CD	LYS		83	84.465	6.827	27.993	1.00 35.16 A
	ATOM	87	CE	LYS		83	85.465	5.683	27.945	1.00 39.06 A
	ATOM	88	NZ	LYS		83	85.512	4.974	29.266	1.00 41.00 A
	ATOM	89	C	LYS		83	81.462	7.775	25.998	1.00 22.51 A
	ATOM	90	Ö		A	83	82.324	7.677	25.120	1.00 23.24 A
20	ATOM	91	N	PHE		84	80.800	8.907	26.227	1.00 20.27 A
20	ATOM	92	CA	PHE		84	81.118	10.098	25.454	1.00 19.31 A
	ATOM	93	CB	PHE		84	80.016	11.145	25.605	1.00 19.31 A
	ATOM	93	CG	PHE		84	78.683	10.694	25.075	1.00 19.95 A
		95								
25	ATOM	95	CD1	PHE		84	77.855	9.879	25.835	1.00 21.62 A
23	ATOM		CD2	PHE		84	78.278	11.035	23.804	1.00 20.47 A
	ATOM	97	CE1	PHE		84	76.665	9.418	25.339	1.00 19.26 A
	ATOM	98	CE2		A	84	77.073	10.568	23.300	1.00 18.97 A
	ATOM	99	CZ	PHE		84	76.276	9.764	24.068	1.00 19.78 A
20	MOTA	100	C	PHE		84	82.463	10.680	25.863	1.00 19.58 A
30	ATOM	101	0	PHE		84	82.888	10.540	26.998	1.00 20.60 A
	MOTA	102	N	GLY		85	83.141	11.307	24.913	1.00 19.33 A
	MOTA	103	CA	GLY		85	84.434	11.909	25.169	1.00 18.23 A
	MOTA	104	C	GLY		85	84.480	13.368	24.743	1.00 19.96 A
	ATOM	105	0	GLY		85	83.533	14.124	24.962	1.00 20.02 A
35	MOTA	106	N	LYS	A	86	85.568	13.764	24.101	1.00 20.79 A
	MOTA	107	CA	LYS		86	85.736	15.159	23.704	1.00 22.45 A
	MOTA	108	CB	LYS		86	87.168	15.400	23.210	1.00 22.06 A
	MOTA	109	CG	LYS		86	87.399	15.048	21.751	1.00 23.37 A
	MOTA	110	CD		A	86	88.832	14.591	21.505	1.00 26.45 A
40	MOTA	111	CE	LYS		86	89.451	15.275	20.294	1.00 30.25 A
	MOTA	112	NZ	LYS		86	89.771	16.721	20.553	1.00 33.08 A
	MOTA	113	С	LYS	A	86	84.750	15.668	22.661	1.00 21.50 A
	MOTA	114	0		A	86	84.154	14.900	21.916	1.00 21.98 A
	MOTA	115	N	ILE		87	84.582	16.985	22.647	1.00 20.15 A
45	MOTA	116	CA	ILE	A	87	83.712	17.661	21.705	1.00 19.38 A
	MOTA	117	CB	ILE	A	87	83.270	19.037	22.272	1.00 17.37 A
	ATOM	118	CG2	ILE	A	87	82.724	19.935	21.163	1.00 15.07 A
	MOTA	119	CG1	ILE	A	87	82.222	18.800	23.371	1.00 18.62 A
	ATOM	120	CD1	ILE	A	87	81.848	20.025	24.190	1.00 16.91 A
50	MOTA	121	С	ILE	A	87	84.549	17.836	20.436	1.00 19.85 A
	MOTA	122	0	ILE	Α	87	85.666	18.317	20.502	1.00 21.66 A
	MOTA	123	N	LEU	А	88	84.030	17.406	19.293	1.00 19.65 A
	ATOM	124	CA	LEU		88	84.771	17.539	18.047	1.00 20.20 A
	ATOM	125	СВ	LEU		88	84.423	16.405	17.078	1.00 18.76 A
55	ATOM	126	CG	LEU		88	84.807	14.981	17.493	1.00 16.99 A
	ATOM	127		LEU		88	84.122	13.995	16.570	1.00 13.92 A
	ATOM	128	CD2	LEU		88	86.305	14.809	17.441	1.00 11.51 A
	ATOM	129	C	LEU		88	84.429	18.861	17.407	1.00 20.87 A
	ATOM	130	ō	LEU		88	85.233	19.443	16.709	1.00 21.48 A
	111 011	130	0	250	^		00.200	20.773	10.705	1.50 L1.40 A

	ATOM	131	N	GLY	A	89	83.221	19.339	17.639	1.00 22.34 A
	ATOM	132	CA	GLY	A	89	82.856	20.601	17.043	1.00 25.87 A
	ATOM	133	C	GLY	Α	89	81.476	21.057	17.451	1.00 29.45 A
	ATOM	134	ō	GLY		89	80.673	20.292	17.990	1.00 29.48 A
5	ATOM	135	N	GLU		90	81.196	22.321	17.188	1.00 32.71 A
,										
	MOTA	136	CA	GLU		90	79.904	22.864	17.530	1.00 37.61 A
	ATOM	137	CB	GLU		90	80.047	23.798	18.738	1.00 38.05 A
	ATOM	138	CG	GLU		90	80.123	22.998	20.037	1.00 42.04 A
	ATOM	139	CD	GLU	A	90	80.463	23.813	21.270	1.00 45.47 A
10	ATOM	140	OE1	GLU	A	90	81.662	24.137	21.477	1.00 47.26 A
	ATOM	141	OE2	GLU	А	90	79.524	24.119	22.041	1.00 47.39 A
	ATOM	142	С	GLU		90	79.277	23.565	16.349	1.00 40.01 A
	ATOM	143	ŏ	GLU		90	79.972	24.148	15.518	1.00 42.05 A
	MOTA	144	N	GLY		91	77.962	23.440	16.240	1.00 42.05 A
15	MOTA	145	CA	GLY		91	77.238	24.102	15.174	1.00 43.15 A
	MOTA	146	C	GLY		91	76.276	25.035	15.892	1.00 45.06 A
	MOTA	147	0	GLY	Α	91	76.317	25.149	17.134	1.00 43.58 A
	MOTA	148	N	SER	A	92	75.408	25.699	15.136	1.00 46.66 A
	ATOM	149	CA	SER	A	92	74.430	26.606	15.742	1.00 48.21 A
20	ATOM	150	CB	SER	Α	92	73.754	27.462	14.660	1.00 51.13 A
	ATOM	151	OG	SER		92	73.601	26.741	13.439	1.00 54.79 A
	ATOM	152	c	SER		92	73.382	25.827	16.538	1.00 47.10 A
	ATOM	153		SER		92	73.055	26.190	17.678	1.00 47.10 A
			0							
	MOTA	154	N	PHE		93	72.874	24.743	15.957	1.00 44.39 A
25	MOTA	155	CA	PHE		93	71.866	23.942	16.648	1.00 41.99 A
	MOTA	156	CB	PHE	A	93	70.617	23.798	15.780	1.00 43.92 A
	ATOM	157	CG	PHE	A	93	70.434	24.919	14.814	1.00 47.66 A
	ATOM	158	CD1	PHE	A	93	70.689	24.729	13.455	1.00 49.35 A
	ATOM	159	CD2	PHE	Α	93	70.061	26.185	15.264	1.00 49.16 A
30	ATOM	160		PHE		93	70.581	25.789	12.551	1.00 51.11 A
	ATOM	161	CE2	PHE		93	69.949	27.257	14.374	1.00 50.58 A
	ATOM	162	CZ	PHE		93	70.209	27.062	13.014	1.00 51.37 A
			C	PHE		93				1.00 31.37 A
	MOTA	163					72.352	22.555	17.028	
	MOTA	164	0	PHE		93	71.532	21.670	17.257	1.00 38.33 A
35	MOTA	165	N	SER		94	73.665	22.351	17.106	1.00 33.28 A
	ATOM	166	CA	SER	A	94	74.151	21.028	17.440	1.00 29.57 A
	MOTA	167	CB	SER	A	94	73.996	20.106	16.227	1.00 30.45 A
	ATOM	168	OG	SER	A	94	75.123	20.190	15.368	1.00 30.51 A
	ATOM	169	C	SER	A	94	75.588	20.952	17.936	1.00 27.66 A
40	ATOM	170	0	SER		94	76.369	21.893	17.803	1.00 27.25 A
	ATOM	171	N	THR		95	75.927	19.807	18.512	1.00 25.06 A
	ATOM	172	CA	THR		95	77.264	19.572	19.027	1.00 23.70 A
						95				
	ATOM	173	CB	THR			77.310	19.626	20.582	
	MOTA	174		THR		95	76.801	20.886	21.044	1.00 25.68 A
45	ATOM	175		THR		95	78.731	19.458	21.073	1.00 22.92 A
	MOTA	176	C	THR	A	95	77.655	18.180	18.594	1.00 22.05 A
	MOTA	177	0	THR	A	95	76.860	17.250	18.673	1.00 21.43 A
	ATOM	178	N	VAL	A	96	78.883	18.029	18.129	1.00 21.52 A
	MOTA	179	CA	VAL	A	96	79.348	16.723	17.702	1.00 19.53 A
50	ATOM	180	CB	VAL		96	79.980	16.818	16.316	1.00 19.24 A
50	ATOM	181		VAL		96	80.418	15.443	15.839	1.00 17.73 A
						96			15.353	
	MOTA	182		VAL			78.983	17.442		1.00 18.03 A
	MOTA	183	С	VAL		96	80.364	16.242	18.722	1.00 19.43 A
	MOTA	184	0	VAL		96	81.372	16.910	18.959	1.00 19.84 A
55	MOTA	185	N	VAL		97	80.099	15.082	19.324	1.00 17.90 A
	ATOM	186	CA	VAL		97	80.989	14.532	20.341	1.00 17.32 A
	MOTA	187	CB	VAL		97	80.283	14.438	21.736	1.00 18.35 A
	ATOM	188	CG1	VAL	Α	97	79.581	15.750	22.066	1.00 20.10 A
	ATOM	189	CG2	VAL	Α	97	79.234	13.357	21.713	1.00 23.78 A

	ATOM	190				97	01 431	12 144	19.949	1.00 17.15 A
	ATOM	191	C	VAL		97	81.471 80.727	13.144	19.379	1.00 17.13 A
						98				
	MOTA	192	N	LEU			82.735	12.866	20.243	1.00 17.34 A
-	ATOM	193	CA	LEU		98	83.331	11.575	19.974	1.00 17.44 A
5	ATOM	194	CB	LEU		98	84.853	11.689	19.990	1.00 17.84 A
	MOTA	195	CG	LEU		98	85.656	10.407	19.737	1.00 18.59 A
	MOTA	196		LEU		98	85.259	9.803	18.387	1.00 18.87 A
	MOTA	197		LEU		98	87.151	10.738	19.772	1.00 16.62 A
	MOTA	198	C	LEU		98	82.874	10.626	21.081	1.00 18.35 A
10	MOTA	199	0	LEU		98	82.992	10.926	22.259	1.00 18.60 A
	MOTA	200	N	ALA		99	82.340	9.476	20.697	1.00 19.15 A
	ATOM	201	CA	ALA		99	81.888	8.513	21.675	1.00 19.73 A
	MOTA	202	CB	ALA		99	80.383	8.534	21.759	1.00 17.97 A
	MOTA	203	С	ALA		99	82.360	7.117	21.317	1.00 21.86 A
15	MOTA	204	0	ALA		99	82.502	6.766	20.131	1.00 22.18 A
	MOTA	205	N	ARG	Α	100	82.631	6.324	22.345	1.00 21.93 A
	MOTA	206	CA	ARG	Α	100	83.025	4.963	22.102	1.00 23.29 A
	ATOM	207	CB	ARG	Α	100	84.333	4.637	22.805	1.00 25.99 A
	ATOM	208	CG	ARG	Α	100	84.870	3.271	22.388	1.00 31.56 A
20	ATOM	209	CD	ARG	Α	100	86.146	2.923	23.129	1.00 35.19 A
	ATOM	210	NE	ARG	Α	100	87.220	3.875	22.847	1.00 37.39 A
	ATOM	211	CZ	ARG	Α	100	87.958	3.870	21.740	1.00 38.05 A
	ATOM	212	NH1	ARG	Α	100	87.742	2.953	20.797	1.00 37.25 A
	ATOM	213	NH2	ARG	Α	100	88.918	4.780	21.580	1.00 36.22 A
25	ATOM	214	C	ARG	Α	100	81.904	4.060	22.603	1.00 22.07 A
	ATOM	215	0	ARG	Α	100	81.460	4.177	23.743	1.00 22.10 A
	ATOM	216	N	GLU			81.417	3.189	21.734	1.00 21.29 A
	ATOM	217	CA	GLU	А	101	80.357	2.262	22.119	1.00 22.87 A
	ATOM	218	CB	GLU	А	101	79.747	1.631	20.867	1.00 23.10 A
30	ATOM	219	CG	GLU		101	78.740	0.563	21.148	1.00 22.71 A
	ATOM	220	CD	GLU			78.128	0.040	19.878	1.00 23.56 A
	ATOM	221		GLU			78.892	-0.198	18.922	1.00 21.84 A
	ATOM	222	OE2	GLU			76.890	-0.143	19.832	1.00 26.29 A
	ATOM	223	C	GLU			80.942	1.176	23.037	1.00 21.56 A
35	ATOM	224	ō	GLU			81.884	0.485	22.666	1.00 20.69 A
	ATOM	225	N	LEU			80.389	1.042	24.236	1.00 21.11 A
	ATOM	226	CA	LEU			80.874	0.057	25.204	1.00 21.54 A
	ATOM	227	CB	LEU		102	80.075	0.199	26.507	1.00 20.90 A
	ATOM	228	CG	LEU			80.193	1.620	27.092	1.00 22.35 A
40	ATOM	229		LEU			79.177	1.798	28.207	1.00 20.18 A
	ATOM	230		LEU			81.600	1.866	27.608	1.00 17.47 A
	ATOM	231	C	LEU			80.896	-1.415	24.729	1.00 20.27 A
	ATOM	232	o	LEU			81.922	-2.078	24.825	1.00 21.63 A
	ATOM	233	N	ALA			79.792	-1.922	24.201	1.00 18.37 A
45	ATOM	234	CA	ALA			79.757	-3.307	23.731	1.00 20.54 A
75	ATOM	235	CB	ALA			78.333	-3.694	23.359	1.00 19.31 A
	ATOM	236	С	ALA			80.688	-3.658	22.552	1.00 19.31 A
	ATOM	237	0	ALA			81.002	-4.829	22.358	1.00 22.20 A
	ATOM	238	N	THR			81.141	-2.677	21.775	1.00 20.79 A
50	ATOM	239	CA	THR		104	81.972	-2.999	20.622	1.00 20.79 A
50										
	ATOM	240 241	CB OC1	THR			81.279 81.174	-2.632	19.326	1.00 20.97 A 1.00 23.21 A
	ATOM							-1.205	19.259	
	ATOM	242	CG2				79.891	-3.266	19.245	1.00 19.82 A
	ATOM	243	C	THR		104	83.304	-2.300	20.569	1.00 23.57 A
55	ATOM	244	0	THR			84.168	-2.687	19.796	1.00 23.41 A
	ATOM	245	N	SER		105	83.454	-1.243	21.359	1.00 24.64 A
	ATOM	246	CA	SER		105	84.687	-0.487	21.390	1.00 24.23 A
	ATOM	247	CB	SER			85.855	-1.467	21.481	1.00 25.40 A
	MOTA	248	OG	SER	Α	105	87.074	-0.788	21.719	1.00 34.15 A

	ATOM	249	C	SER	Α	105	84.819	0.454	20.163	1.00 23.42 A
	ATOM	250	0	SER	А	105	85.803	1.187	20.013	1.00 23.28 A
	ATOM	251	N	ARG	Α	106	83.821	0.448	19.295	1.00 21.19 A
	ATOM	252	CA	ARG			83.850	1.323	18.115	1.00 22.25 A
5	ATOM	253	CB	ARG			82.754	0.922	17.118	1.00 24.82 A
,	ATOM	254	CG	ARG			83.027	-0.343	16.349	1.00 25.20 A
		255	CD	ARG			81.740	-0.942	15.884	1.00 25.20 A
	ATOM									
	ATOM	256	NE	ARG			81.972	-1.900	14.815	1.00 26.11 A
10	ATOM	257	CZ	ARG			81.042	-2.707	14.322	1.00 24.24 A
10	MOTA	258		ARG			79.805	-2.677	14.818	1.00 21.06 A
	MOTA	259		ARG			81.351	-3.513	13.315	1.00 20.25 A
	ATOM	260	C	ARG			83.655	2.806	18.433	1.00 19.79 A
	MOTA	261	0	ARG			82.836	3.175	19.266	1.00 18.73 A
	ATOM	262	N	GLU	Α	107	84.404	3.646	17.736	1.00 19.82 A
15	MOTA	263	CA	GLU	Α	107	84.294	5.086	17.903	1.00 21.14 A
	ATOM	264	CB	GLU	Α	107	85.656	5.746	17.777	1.00 21.88 A
	ATOM	265	CG	GLU	Α	107	86.562	5.428	18.926	1.00 26.09 A
	ATOM	266	CD	GLU	Α	107	87.916	6.043	18.746	1.00 30.29 A
	ATOM	267	OE1	GLU	Α	107	88.212	7.057	19.434	1.00 32.48 A
20	ATOM	268	OE2	GLU	А	107	88.678	5.512	17.901	1.00 31.98 A
	ATOM	269	C	GLU	А	107	83.358	5.693	16.870	1.00 20.50 A
	ATOM	270	o	GLU			83.474	5.429	15.676	1.00 20.70 A
	ATOM	271	N	TYR			82.415	6.498	17.347	1.00 20.38 A
	ATOM	272	CA	TYR			81.464	7.172	16.477	1.00 18.49 A
25	ATOM	273	CB	TYR			80.049	6.660	16.700	1.00 17.92 A
20	ATOM	274	CG	TYR			79.828	5.247	16.238	1.00 23.37 A
	ATOM	275		TYR			79.528	4.964	14.886	1.00 23.37 A
	ATOM	276	CE1	TYR			79.357	3.648	14.458	1.00 22.79 A
	ATOM	277		TYR			79.820	4.180	17.154	
30										
30	ATOM	278	CE2	TYR			79.583	2.873	16.740	1.00 20.43 A
	MOTA	279	CZ	TYR			79.346	2.609	15.392	1.00 23.44 A
	MOTA	280	OH	TYR			79.061	1.321	14.972	1.00 24.10 A
	MOTA	281	С	TYR			81.478	8.635	16.828	1.00 18.53 A
	MOTA	282	0	TYR			81.778	9.011	17.971	1.00 17.37 A
35	ATOM	283	N	ALA.			81.169	9.453	15.829	1.00 17.24 A
	ATOM	284	CA	ALA .			81.053	10.885	16.006	1.00 15.98 A
	MOTA	285	CB	ALA			81.597	11.600	14.788	1.00 15.20 A
	MOTA	286	С	ALA .	Α	109	79.528	11.087	16.140	1.00 15.73 A
	MOTA	287	0	ALA.	Α	109	78.767	10.873	15.191	1.00 15.79 A
40	MOTA	288	N	ILE.	Α	110	79.070	11.474	17.320	1.00 14.95 A
	ATOM	289	CA	ILE.	Α	110	77.636	11.636	17.511	1.00 15.99 A
	MOTA	290	CB	ILE	Α	110	77.188	10.940	18.815	1.00 15.51 A
	ATOM	291	CG2	ILE	А	110	75.697	11.126	19.039	1.00 14.44 A
	ATOM	292	CG1	ILE .	Α	110	77.541	9.452	18.729	1.00 16.63 A
45	ATOM	293	CD1	ILE	А	110	76.964	8.595	19.847	1.00 16.83 A
	ATOM	294	C	ILE			77.176	13.085	17.514	1.00 16.55 A
	ATOM	295	o	ILE			77.583	13.873	18.370	1.00 16.24 A
	ATOM	296	N	LYS			76.343	13.430	16.538	1.00 16.03 A
	ATOM	297	CA	LYS			75.804	14.777	16.430	1.00 18.21 A
50	ATOM	298	CB	LYS			75.341	15.065	14.997	1.00 19.36 A
50	ATOM	299	CG	LYS			75.035	16.548	14.768	1.00 22.68 A
	ATOM	300	CD	LYS			74.461	16.844	13.396	1.00 22.68 A
	ATOM	301	CE	LYS			74.461	18.222	12.930	1.00 23.87 A
			NZ							
55	ATOM	302		LYS			73.744	18.938	12.304	1.00 28.83 A
23	MOTA	303	C	LYS			74.608	14.866	17.383	1.00 17.40 A
	ATOM	304	0	LYS			73.646	14.115	17.239	1.00 18.27 A
	MOTA	305	N	ILE		112	74.672	15.781	18.344	1.00 15.41 A
	MOTA	306	CA	ILE			73.609	15.938	19.331	1.00 16.56 A
	ATOM	307	CB	ILE	Α	112	74.194	15.819	20.777	1.00 17.09 A

	MOTA	308	CG2	ILE A	112	73.073	15.926	21.830	1.00 11.60 A
	ATOM	309	CG1	ILE A	112	74.957	14.480	20.885	1.00 16.81 A
	ATOM	310	CD1	ILE A	112	75.771	14.262	22.178	1.00 15.96 A
	ATOM	311	C	ILE A		72.876	17.261	19.158	1.00 17.98 A
5	ATOM	312	ō	ILE A		73.504	18.314	18.965	1.00 16.70 A
-	ATOM	313	N	LEU /		71.546	17.198	19.195	1.00 19.61 A
	ATOM	314	CA	LEU A		70.711	18.393	19.034	1.00 19.01 A
	ATOM	315	CB	LEU A		70.058	18.434	17.641	1.00 22.17 A
	MOTA	316	CG	LEU A		70.906	18.273	16.367	1.00 22.83 A
10	MOTA	317		LEU A		71.124	16.792	16.059	1.00 22.72 A
	MOTA	318		LEU A		70.191	18.912	15.206	1.00 21.97 A
	ATOM	319	С	LEU A		69.612	18.419	20.088	1.00 24.22 A
	MOTA	320	0	LEU A		69.062	17.378	20.469	1.00 24.61 A
	ATOM	321	N	GLU A	114	69.285	19.615	20.559	1.00 27.06 A
15	MOTA	322	CA	GLU A	114	68.247	19.759	21.567	1.00 28.93 A
	ATOM	323	CB	GLU A	114	68.586	20.926	22.488	1.00 31.39 A
	ATOM	324	CG	GLU A	114	67.671	21.026	23.684	1.00 39.92 A
	ATOM	325	CD	GLU A	114	67.676	22.406	24.300	1.00 45.42 A
	ATOM	326		GLU Z		67.160	23.356	23.655	1.00 46.90 A
20	ATOM	327	OE2	GLU A		68.204	22.540	25.429	1.00 50.09 A
	ATOM	328	C	GLU A		66.887	19.978	20.892	1.00 29.21 A
	ATOM	329	o	GLU A		66.679	20.969	20.177	1.00 29.53 A
	ATOM	330	N	LYS A		65.962	19.051	21.116	1.00 28.74 A
	ATOM	331	CA	LYS A		64.642	19.152	20.507	1.00 29.44 A
25	ATOM	332		LYS A			18.002	20.307	1.00 29.44 A
23			CB			63.744			
	ATOM	333	CG	LYS A		63.827	16.758	20.103	1.00 28.47 A
	MOTA	334	CD	LYS A		63.026	15.571	20.639	1.00 27.07 A
	MOTA	335	CE	LYS A		63.738	14.854	21.779	1.00 28.88 A
	MOTA	336	NZ	LYS A		62.963	13.672	22.282	1.00 26.42 A
30	MOTA	337	C	LYS A		63.947	20.502	20.724	1.00 29.72 A
	MOTA	338	0	LYS A		63.310	21.025	19.799	1.00 30.03 A
	ATOM	339	N	ALA A		64.082	21.091	21.910	1.00 28.83 A
	MOTA	340	CA	ALA A		63.407	22.365	22.159	1.00 29.91 A
	ATOM	341	CB	ALA A	116	63.470	22.749	23.647	1.00 28.16 A
35	ATOM	342	C	ALA A	116	63.976	23.480	21.311	1.00 30.93 A
	ATOM	343	0	ALA A	116	63.231	24.217	20.667	1.00 32.28 A
	ATOM	344	N	HIS A	117	65.297	23.593	21.292	1.00 31.66 A
	ATOM	345	CA	HIS A	117	65.951	24.645	20.523	1.00 32.13 A
	ATOM	346	CB	HIS A		67.472	24.571	20.728	1.00 34.12 A
40	ATOM	347	CG	HIS A		68.219	25.741	20.169	1.00 37.74 A
	ATOM	348		HIS A		67.794	26.959	19.761	1.00 39.67 A
	ATOM	349		HIS A		69.582	25.727	19.966	1.00 42.04 A
	ATOM	350		HIS A		69.965	26.884	19.454	1.00 42.04 A
	ATOM	351		HIS A		68.899	27.649	19.320	1.00 40.56 A
45		352	C						1.00 40.36 A
43	ATOM			HIS A		65.600	24.547	19.040	
	ATOM	353	0	HIS A		65.466	25.560	18.350	1.00 32.37 A
	MOTA	354	N	ILE A		65.430	23.330	18.544	1.00 30.26 A
	MOTA	355	CA	ILE A		65.102	23.158	17.132	1.00 29.28 A
	MOTA	356	CB	ILE A		65.266	21.696	16.712	1.00 27.64 A
50	MOTA	357		ILE A		64.560	21.439	15.401	1.00 22.46 A
	ATOM	358		ILE A		66.756	21.371	16.642	1.00 27.22 A
	ATOM	359		ILE A		67.036	19.917	16.437	1.00 30.51 A
	MOTA	360	C	ILE A	118	63.688	23.618	16.816	1.00 30.41 A
	MOTA	361	0	ILE A	118	63.444	24.251	15.785	1.00 29.55 A
55	MOTA	362	N	ILE A	119	62.756	23.291	17.705	1.00 29.59 A
	ATOM	363	CA	ILE A	119	61.376	23.682	17.497	1.00 29.18 A
	ATOM	364	CB	ILE A		60.447	22.979	18.506	1.00 27.15 A
	ATOM	365		ILE A		59.071	23.623	18.486	1.00 22.69 A
	ATOM	366		ILE A		60.394	21.486	18.173	1.00 23.45 A

	ATOM	367	CD1	ILE A	. 119	59.666	20.665	19.173	1.00 19.08 A
	ATOM	368	C	ILE A	. 119	61.223	25.194	17.617	1.00 30.65 A
	ATOM	369	0	ILE A	119	60.574	25.832	16.786	1.00 30.59 A
	ATOM	370	N	ALA A	120	61.837	25.768	18.642	1.00 31.95 A
5	ATOM	371	CA	ALA A	120	61.752	27.205	18.848	1.00 33.69 A
	ATOM	372	CB	ALA A	120	62.473	27.608	20.150	1.00 33.17 A
	ATOM	373	C	ALA A		62.330	27.973	17.671	1.00 34.80 A
	ATOM	374	0	ALA A		61.865	29.067	17.362	1.00 37.34 A
	ATOM	375	N	GLU A		63.328	27.413	16.997	1.00 35.09 A
10	ATOM	376	CA	GLU A		63.941	28.116	15.872	1.00 35.31 A
	ATOM	377	CB	GLU A		65.453	27.927	15.933	1.00 39.72 A
	ATOM	378	CG	GLU A		66.103	28.735	17.038	1.00 45.91 A
	ATOM	379	CD	GLU A		65.955	30.225	16.784	1.00 49.51 A
	ATOM	380		GLU A		66.634	30.736	15.866	1.00 52.87 A
15	ATOM	381	OE2	GLU A		65.148	30.879	17.482	1.00 51.35 A
13	ATOM	382	C	GLU A		63.421	27.699	14.499	1.00 31.33 A
	ATOM	383	0	GLU A		63.964	28.109	13.468	1.00 31.41 A
	ATOM	384	N	ASN A		62.363	26.891	14.497	1.00 31.41 A
	ATOM	385	CA	ASN A		61.771	26.367	13.266	1.00 33.86 A
20						61.112			
20	ATOM	386	CB	ASN A			27.473	12.464	
	MOTA	387		ASN A		59.962	28.081	13.193	1.00 39.62 A
	ATOM	388				60.148	28.788	14.185	1.00 39.90 A
	ATOM	389		ASN A		58.753	27.794	12.727	1.00 41.02 A
2.5	MOTA	390	С	ASN A		62.798	25.686	12.397	1.00 31.78 A
25	ATOM	391	0	ASN A		62.958	26.035	11.230	1.00 32.05 A
	MOTA	392	N	LYS A		63.494	24.714	12.965	1.00 28.71 A
	ATOM	393	CA	LYS A		64.508	24.008	12.217	1.00 29.39 A
	MOTA	394	CB	LYS A		65.842	24.036	12.974	1.00 31.70 A
	MOTA	395	CG	LYS A		66.434	25.416	13.132	1.00 33.49 A
30	MOTA	396	CD	LYS A		66.612	26.076	11.763	1.00 37.43 A
	MOTA	397	CE	LYS A		67.174	27.491	11.898	1.00 38.52 A
	ATOM	398	NZ	LYS A		67.337	28.176	10.582	1.00 37.85 A
	ATOM	399	C	LYS A		64.116	22.572	11.931	1.00 28.30 A
	ATOM	400	0	LYS A		64.867	21.844	11.289	1.00 29.68 A
35	MOTA	401	N	VAL A		62.944	22.162	12.404	1.00 26.80 A
	ATOM	402	CA	VAL A		62.484	20.796	12.175	1.00 26.73 A
	ATOM	403	CB	VAL A		61.024	20.593	12.622	1.00 26.31 A
	ATOM	404		VAL A		60.532	19.222	12.191	1.00 25.31 A
	ATOM	405	CG2	VAL A		60.918	20.720	14.134	1.00 26.73 A
40	ATOM	406	C	VAL A		62.594	20.351	10.722	1.00 27.11 A
	ATOM	407	0	VAL A		62.973	19.218	10.450	1.00 29.79 A
	ATOM	408	N	PRO A	125	62.270	21.228	9.763	1.00 27.28 A
	ATOM	409	CD	PRO A		61.610	22.544	9.818	1.00 27.49 A
	ATOM	410	CA	PRO A	125	62.386	20.758	8.378	1.00 27.41 A
45	ATOM	411	CB	PRO A	125	61.775	21.904	7.563	1.00 26.08 A
	MOTA	412	CG	PRO A	125	60.821	22.546	8.524	1.00 27.54 A
	ATOM	413	С	PRO A	125	63.837	20.506	8.006	1.00 27.90 A
	ATOM	414	0	PRO A	125	64.162	19.572	7.260	1.00 26.27 A
	ATOM	415	N	TYR A	126	64.703	21.350	8.550	1.00 28.64 A
50	ATOM	416	CA	TYR A	126	66.123	21.271	8.288	1.00 30.11 A
	ATOM	417	CB	TYR A	126	66.791	22.528	8.809	1.00 36.70 A
	ATOM	418	CG	TYR A	126	66.440	23.774	8.013	1.00 44.64 A
	ATOM	419		TYR A	126	66.984	23.988	6.744	1.00 47.43 A
	ATOM	420		TYR A		66.737	25.173	6.037	1.00 50.16 A
55	ATOM	421	CD2	TYR A		65.620	24.774	8.557	1.00 47.03 A
	ATOM	422	CE2	TYR A		65.369	25.955	7.861	1.00 49.52 A
	ATOM	423	CZ	TYR A		65.936	26.152	6.605	1.00 50.60 A
	ATOM	424	OH	TYR A		65.754	27.349	5.941	1.00 52.77 A
	ATOM	425	C	TYR A		66.794	20.041	8.874	1.00 28.69 A

	ATOM	426	0	TYR A		67.613	19.407	8.208	1.00 28.32 A
	ATOM	427	N	VAL A		66.464	19.714	10.118	1.00 25.64 A
	ATOM	428	CA	VAL A	. 127	67.033	18.550	10.766	1.00 24.89 A
	ATOM	429	CB	VAL A	. 127	66.664	18.513	12.258	1.00 26.70 A
5	ATOM	430	CG1	VAL A	127	67.158	17.206	12.881	1.00 22.51 A
	ATOM	431	CG2	VAL A	127	67.255	19.743	12.972	1.00 23.84 A
	ATOM	432	C	VAL A	127	66.521	17.276	10.097	1.00 24.81 A
	ATOM	433	0	VAL A		67.260	16.315	9.890	1.00 24.02 A
	ATOM	434	N	THR A		65.245	17.290	9.755	1.00 24.02 A
10	ATOM	435	CA	THR A		64.608	16.164	9.088	1.00 24.59 A
	ATOM	436	CB	THR A		63.123	16.471	8.843	1.00 25.38 A
	ATOM	437		THR A		62.478	16.652	10.106	1.00 25.76 A
	ATOM	438		THR A		62.451	15.354	8.066	1.00 22.88 A
	ATOM	439	C	THR A		65.266	15.875	7.744	1.00 24.53 A
15	ATOM	440	ō	THR A		65.560	14.729	7.426	1.00 25.53 A
13	ATOM	441	N	ARG A		65.477	16.925	6.957	1.00 24.82 A
	ATOM	442	CA	ARG A		66.099	16.812	5.646	1.00 25.49 A
	ATOM	443	CB	ARG A		66.111	18.181	4.959	1.00 26.78 A
	MOTA	444	CG	ARG A		66.648	18.175	3.529	1.00 32.33 A
20	MOTA	445	CD	ARG A		66.579	19.563	2.878	1.00 36.93 A
	MOTA	446	NE	ARG A		65.326	20.249	3.184	1.00 42.70 A
	MOTA	447	CZ	ARG A		65.254	21.462	3.730	1.00 46.67 A
	ATOM	448		ARG A		66.366	22.128	4.018	1.00 48.50 A
	ATOM	449		ARG A		64.073	21.997	4.027	1.00 48.90 A
25	ATOM	450	C	ARG A	. 129	67.532	16.296	5.801	1.00 26.46 A
	MOTA	451	0	ARG A		68.002	15.456	5.020	1.00 24.76 A
	MOTA	452	N	GLU A	130	68.216	16.795	6.825	1.00 25.56 A
	MOTA	453	CA	GLU A	130	69.582	16.393	7.076	1.00 28.29 A
	ATOM	454	CB	GLU A	130	70.118	17.106	8.310	1.00 27.95 A
30	ATOM	455	CG	GLU A	130	71.591	16.875	8.539	1.00 29.48 A
	ATOM	456	CD	GLU A	130	72.107	17.566	9.787	1.00 32.14 A
	ATOM	457	OE1	GLU A		71.297	18.221	10.483	1.00 32.67 A
	ATOM	458	OE2	GLU A		73.325	17.450	10.069	1.00 32.21 A
	ATOM	459	С	GLU A		69.665	14.886	7.279	1.00 29.86 A
35	ATOM	460	ō	GLU A		70.498	14.200	6.668	1.00 29.35 A
	ATOM	461	N	ARG A		68.797	14.382	8.150	1.00 30.84 A
	ATOM	462	CA	ARG A		68.763	12.966	8.451	1.00 31.62 A
	ATOM	463	CB	ARG A		67.786	12.684	9.598	1.00 33.12 A
	ATOM	464	CG	ARG A		67.557	11.190	9.831	1.00 36.17 A
40	ATOM	465	CD	ARG A		66.560	10.925	10.946	1.00 41.69 A
40	ATOM	466	NE	ARG A		66.330	9.492	11.166	1.00 46.62 A
	ATOM	467	CZ	ARG A		65.692	8.986	12.224	1.00 48.29 A
	ATOM	468		ARG A		65.215	9.795	13.165	1.00 49.51 A
		469		ARG A		65.544	7.671	12.352	1.00 49.31 A
45	ATOM								
43	ATOM	470	С	ARG A		68.371	12.138	7.235	1.00 30.59 A
	MOTA	471	0	ARG A		68.897	11.051	7.026	1.00 29.96 A
	ATOM	472	N	ASP A		67.446	12.649	6.433	1.00 29.54 A
	ATOM	473	CA	ASP A		67.000	11.913	5.259	1.00 29.40 A
	MOTA	474	CB	ASP A		65.735	12.565	4.708	1.00 32.43 A
50	MOTA	475	CG	ASP A		64.531	12.395	5.655	1.00 38.15 A
	MOTA	476		ASP A		64.749	12.227	6.881	1.00 40.40 A
	ATOM	477	OD2	ASP A		63.365	12.439	5.186	1.00 41.19 A
	ATOM	478	C	ASP A		68.088	11.789	4.189	1.00 27.62 A
	ATOM	479	0	ASP A	. 132	68.232	10.744	3.553	1.00 26.54 A
55	ATOM	480	N	VAL A	. 133	68.862	12.850	4.011	1.00 25.14 A
	ATOM	481	CA	VAL A	133	69.939	12.857	3.044	1.00 24.12 A
	ATOM	482	CB	VAL A	. 133	70.451	14.272	2.833	1.00 24.07 A
	ATOM	483	CG1	VAL A		71.802	14.247	2.143	1.00 23.77 A
	ATOM	484		VAL A		69.461	15.030	2.008	1.00 24.30 A

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	MOTA	485	C	VAL			71.099	11.975	3.504	1.00 24.97 A
	ATOM	486	0	VAL			71.672	11.221	2.712	1.00 24.95 A
	MOTA	487	N	MET			71.458	12.074	4.779	1.00 23.41 A
	MOTA	488	CA	MET			72.539	11.255	5.268	1.00 23.12 A
5	MOTA	489	CB	MET			72.932	11.653	6.683	1.00 21.12 A
	MOTA	490	CG	MET			73.608	13.005	6.759	1.00 21.21 A
	ATOM	491	SD	MET	Α	134	74.530	13.204	8.291	1.00 20.52 A
	ATOM	492	CE	MET	Α	134	73.172	13.347	9.534	1.00 17.71 A
	ATOM	493	C	MET	Α	134	72.163	9.783	5.237	1.00 24.75 A
10	MOTA	494	0	MET	Α	134	73.027	8.918	5.039	1.00 25.73 A
	ATOM	495	N	SER	Α	135	70.885	9.474	5.425	1.00 23.96 A
	ATOM	496	CA	SER	Α	135	70.484	8.064	5.408	1.00 24.82 A
	ATOM	497	CB	SER	Α	135	69.048	7.889	5.917	1.00 24.63 A
	ATOM	498	OG	SER	Α	135	68.139	8.496	5.015	1.00 29.80 A
15	ATOM	499	С	SER	Α	135	70.585	7.479	4.003	1.00 22.35 A
	ATOM	500	0	SER	А	135	70.534	6.274	3.829	1.00 21.60 A
	ATOM	501	N	ARG			70.729	8.335	3.004	1.00 21.91 A
	ATOM	502	CA	ARG			70.815	7.858	1.631	1.00 23.76 A
	ATOM	503	CB	ARG			69.988	8.762	0.714	1.00 25.55 A
20	ATOM	504	CG	ARG			68.500	8.782	1.069	1.00 31.38 A
	ATOM	505	CD	ARG			67.764	9.897	0.332	1.00 33.65 A
	ATOM	506	NE	ARG			68.024	9.809	-1.099	1.00 38.77 A
	ATOM	507	CZ	ARG			67.654	10.718	-1.996	1.00 30.77 A
	ATOM	508		ARG			66.988	11.806	-1.604	1.00 41.27 A
25	ATOM	509		ARG			67.971	10.544	-3.286	1.00 42.33 A
23	ATOM	510	C	ARG			72.248	7.789	1.131	1.00 33.41 A
	ATOM	511	0	ARG			72.520	7.268	0.052	1.00 22.64 A
	ATOM	512	N	LEU			73.168	8.318	1.919	1.00 22.43 A
20	ATOM	513	CA	LEU			74.568	8.307	1.535	1.00 22.60 A
30	ATOM	514	CB	LEU			75.348	9.375	2.308	1.00 20.28 A
	ATOM	515	CG	LEU			74.842	10.793	2.068	1.00 19.72 A
	ATOM	516		LEU			75.695	11.816	2.840	1.00 17.83 A
	MOTA	517		LEU			74.855	11.062	0.564	1.00 18.39 A
	MOTA	518	С	LEU			75.195	6.950	1.775	1.00 22.60 A
35	MOTA	519	0	LEU			75.203	6.445	2.892	1.00 23.75 A
	MOTA	520	N	ASP			75.723	6.371	0.710	1.00 22.09 A
	MOTA	521	CA	ASP			76.383	5.083	0.788	1.00 22.63 A
	MOTA	522	CB	ASP			75.419	3.988	0.340	1.00 25.16 A
40	ATOM	523	CG	ASP			75.976	2.622	0.582	1.00 26.26 A
40	MOTA	524		ASP			76.658	2.480	1.611	1.00 27.29 A
	MOTA	525		ASP			75.740	1.708	-0.237	1.00 30.75 A
	MOTA	526	C	ASP			77.617	5.112	-0.124	1.00 20.82 A
	MOTA	527	0	ASP			77.656	4.445	-1.155	1.00 22.94 A
	MOTA	528	N	HIS			78.612	5.902	0.250	1.00 16.77 A
45	ATOM	529	CA	HIS			79.813	6.050	-0.557	1.00 16.21 A
	MOTA	530	CB	HIS			79.614	7.180	-1.583	1.00 15.30 A
	MOTA	531	CG	HIS			80.755	7.348	-2.534	1.00 16.37 A
	ATOM	532		HIS			80.853	7.087	-3.860	1.00 15.32 A
	ATOM	533	ND1	HIS	Α	139	81.998	7.802	-2.139	1.00 17.12 A
50	MOTA	534	CE1	HIS	Α	139	82.811	7.810	-3.184	1.00 15.92 A
	ATOM	535	NE2	HIS	Α	139	82.140	7.380	-4.238	1.00 13.96 A
	MOTA	536	C	HIS	Α	139	80.985	6.371	0.357	1.00 16.70 A
	ATOM	537	0	HIS	Α	139	80.848	7.116	1.317	1.00 16.89 A
	MOTA	538	N	PRO	Α	140	82.164	5.823	0.056	1.00 16.94 A
55	MOTA	539	CD	PRO	Α	140	82.508	4.991	-1.108	1.00 17.10 A
	MOTA	540	CA	PRO			83.334	6.079	0.895	1.00 17.98 A
	MOTA	541	CB	PRO	Α	140	84.390	5.163	0.291	1.00 17.03 A
	ATOM	542	CG	PRO			84.003	5.114	-1.159	1.00 18.59 A
	ATOM	543	C	PRO			83.822	7.528	1.070	1.00 18.59 A

	ATOM	544	0	PRO	Α	140	84.528	7.817	2.021	1.00 20.11 A
	ATOM	545	N	PHE	Α	141	83.460	8.444	0.179	1.00 19.62 A
	ATOM	546	CA	PHE	Α	141	83.909	9.833	0.345	1.00 18.34 A
	ATOM	547	CB	PHE			84.223	10.474	-1.010	1.00 17.53 A
5	ATOM	548	CG	PHE			85.440	9.880	-1.694	1.00 17.38 A
-	ATOM	549		PHE			86.450	9.275	-0.938	1.00 17.01 A
	ATOM	550	CD2	PHE		141	85.579	9.926	-3.081	1.00 15.76 A
	ATOM	551		PHE			87.572	8.724	-1.550	1.00 16.13 A
	MOTA	552	CE2	PHE			86.707	9.375	-3.708	1.00 16.99 A
10	MOTA	553	CZ	PHE			87.705	8.772	-2.938	1.00 15.01 A
	MOTA	554	C	PHE			82.893	10.680	1.095	1.00 18.14 A
	ATOM	555	0	PHE			83.012	11.896	1.144	1.00 20.74 A
	MOTA	556	N	PHE			81.901	10.037	1.697	1.00 15.85 A
	MOTA	557	CA	PHE	Α	142	80.887	10.761	2.444	1.00 15.95 A
15	ATOM	558	CB	PHE	Α	142	79.558	10.757	1.690	1.00 15.20 A
	ATOM	559	CG	PHE	Α	142	79.507	11.721	0.542	1.00 15.62 A
	ATOM	560	CD1	PHE	А	142	79.295	13.086	0.768	1.00 14.51 A
	ATOM	561	CD2	PHE			79.651	11.265	-0.771	1.00 12.05 A
	ATOM	562	CE1	PHE		142	79.222	13.991	-0.291	1.00 13.97 A
20	ATOM	563	CE2	PHE			79.582	12.157	-1.840	1.00 15.46 A
20	ATOM	564	CZ	PHE			79.365	13.536	-1.601	1.00 14.89 A
	ATOM	565	c	PHE			80.654	10.167	3.824	1.00 15.60 A
	ATOM	566	o	PHE			80.886	8.986	4.061	1.00 15.30 A
			N	VAL			80.182	11.001	4.733	1.00 15.87 A
2.5	MOTA	567								
25	ATOM	568	CA	VAL			79.878	10.564	6.075	1.00 15.04 A
	MOTA	569	CB	VAL			79.304	11.727	6.905	1.00 15.26 A
	MOTA	570		VAL			78.012	12.231	6.276	1.00 11.03 A
	MOTA	571		VAL			79.100	11.296	8.350	1.00 14.40 A
	MOTA	572	C	VAL .			78.828	9.479	5.935	1.00 15.52 A
30	ATOM	573	0	VAL .			78.076	9.453	4.963	1.00 15.45 A
	MOTA	574	N	LYS			78.794	8.580	6.907	1.00 16.29 A
	ATOM	575	CA	LYS	Α	144	77.848	7.482	6.933	1.00 17.45 A
	ATOM	576	CB	LYS	Α	144	78.625	6.150	6.895	1.00 18.05 A
	ATOM	577	CG	LYS	Α	144	77.963	4.967	7.596	1.00 24.34 A
35	ATOM	578	CD	LYS	Α	144	76.922	4.263	6.752	1.00 26.35 A
	ATOM	579	CE	LYS	Α	144	77.461	2.926	6.213	1.00 30.22 A
	ATOM	580	NZ	LYS	А	144	77.576	1.882	7,271	1.00 28.27 A
	ATOM	581	C	LYS	А	144	77.024	7.626	8.222	1.00 17.39 A
	ATOM	582	ō	LYS			77.565	7.913	9.284	1.00 16.92 A
40	ATOM	583	N	LEU			75.711	7.458	8.116	1.00 17.41 A
	ATOM	584	CA	LEU			74.836	7.549	9.274	1.00 18.13 A
	ATOM	585	CB	LEU			73.514	8.210	8.893	1.00 18.86 A
	ATOM	586	CG	LEU			72.612	8.850	9.964	1.00 20.13 A
	ATOM	587		LEU			71.157	8.607	9.582	1.00 20.13 A
45										
43	MOTA	588		LEU			72.900	8.311	11.331	1.00 17.86 A
	MOTA	589	С	LEU			74.559	6.113	9.689	1.00 18.85 A
	MOTA	590	0	LEU			73.905	5.379	8.954	1.00 20.15 A
	MOTA	591	N	TYR			75.030	5.713	10.867	1.00 18.09 A
	MOTA	592	CA	TYR			74.830	4.341	11.329	1.00 15.93 A
50	MOTA	593	CB	TYR	Α	146	76.013	3.871	12.154	1.00 14.52 A
	MOTA	594	CG	TYR			77.295	3.776	11.390	1.00 13.98 A
	ATOM	595	CD1	TYR.	Α	146	78.093	4.907	11.193	1.00 15.01 A
	ATOM	596	CE1	TYR	Α	146	79.329	4.815	10.548	1.00 14.94 A
	ATOM	597		TYR			77.752	2.541	10.912	1.00 14.36 A
55	ATOM	598		TYR			78.984	2.426	10.266	1.00 15.47 A
	ATOM	599	CZ	TYR			79.770	3.566	10.090	1.00 15.70 A
	ATOM	600	OH	TYR			80.999	3.473	9.491	1.00 16.29 A
	ATOM	601	C	TYR			73.591	4.135	12.154	1.00 16.74 A
	ATOM	602	ō	TYR			73.004	3.050	12.132	1.00 17.63 A

	ATOM	603	N	PHE	Α	147	73.198	5.158	12.901	1.00 15.90 A
	ATOM	604	CA	PHE	А	147	72.012	5.041	13.745	1.00 17.10 A
	ATOM	605	CB	PHE		147	72.265	4.057	14.932	1.00 14.80 A
	ATOM	606	CG	PHE		147	73.509	4.366	15.747	1.00 14.00 A
-										
5	ATOM	607		PHE			73.526	5.427	16.657	1.00 15.38 A
	MOTA	608	CD2	PHE	Α	147	74.701	3.663	15.514	1.00 16.83 A
	ATOM	609	CE1	PHE	Α	147	74.709	5.801	17.314	1.00 15.96 A
	ATOM	610	CE2	PHE	А	147	75.907	4.024	16.163	1.00 16.65 A
	ATOM	611	CZ	PHE			75.908	5.107	17.069	1.00 16.96 A
10							71.550	6.378	14.286	1.00 10.30 A
10	MOTA	612	C	PHE						
	ATOM	613	0	PHE			72.225	7.399	14.145	1.00 18.47 A
	ATOM	614	N	THR	Α	148	70.376	6.352	14.897	1.00 19.28 A
	MOTA	615	CA	THR	Α	148	69.801	7.529	15.532	1.00 19.50 A
	ATOM	616	CB	THR	А	148	68.846	8.308	14.597	1.00 19.24 A
15	ATOM	617		THR			67.722	7.485	14.271	1.00 18.29 A
13							69.563	8.727		1.00 18.53 A
	ATOM	618		THR					13.311	
	MOTA	619	С	THR			68.976	7.071	16.718	1.00 19.68 A
	MOTA	620	0	THR	Α	148	68.556	5.915	16.802	1.00 20.20 A
	ATOM	621	N	PHE	Α	149	68.765	7.975	17.653	1.00 20.20 A
20	ATOM	622	CA	PHE	А	149	67.926	7.687	18.797	1.00 20.34 A
	ATOM	623	CB	PHE		149	68.558	6.626	19.728	1.00 19.06 A
			CG							
	MOTA	624		PHE		149	69.932	6.961	20.216	1.00 18.27 A
	MOTA	625		PHE		149	70.114	7.745	21.357	1.00 19.90 A
	MOTA	626	CD2	PHE	Α	149	71.049	6.467	19.559	1.00 19.21 A
25	ATOM	627	CE1	PHE	Α	149	71.387	8.028	21.840	1.00 19.04 A
	ATOM	628	CE2	PHE	А	149	72.341	6.741	20.025	1.00 19.95 A
	MOTA	629	CZ	PHE			72.513	7.520	21,167	1.00 21.19 A
	ATOM	630	C	PHE			67.693	9.004	19.487	1.00 20.94 A
	ATOM	631	0	PHE			68.192	10.035	19.042	1.00 17.91 A
30	ATOM	632	N	GLN			66.888	8.988	20.539	1.00 25.44 A
	ATOM	633	CA	GLN	Α	150	66.609	10.212	21.279	1.00 29.09 A
	ATOM	634	CB	GLN	Α	150	65.518	11.039	20.571	1.00 29.07 A
	ATOM	635	CG	GLN	Δ	150	64.194	10.322	20.309	1.00 31.07 A
	ATOM	636	CD	GLN			63.150	11.227	19.609	1.00 32.52 A
25										
35	MOTA	637		GLN			62.503	12.075	20.243	1.00 30.50 A
	ATOM	638	NE2	GLN			63.009	11.056	18.294	1.00 29.34 A
	MOTA	639	С	GLN	Α	150	66.190	9.927	22.707	1.00 29.59 A
	ATOM	640	0	GLN	Α	150	65.738	8.832	23.018	1.00 30.34 A
	MOTA	641	N	ASP	Α	151	66.407	10.892	23.590	1.00 31.52 A
40	ATOM	642	CA	ASP			65.957	10.750	24.967	1.00 32.22 A
	ATOM	643	CB	ASP			67.093	10.948	25.974	1.00 31.30 A
	MOTA	644	CG	ASP			67.832	12.246	25.790	
	ATOM	645		ASP			67.241	13.217	25.263	1.00 34.30 A
	MOTA	646	OD2	ASP	Α	151	69.011	12.290	26.195	1.00 32.02 A
45	ATOM	647	С	ASP	Α	151	64.914	11.858	25.063	1.00 33.56 A
	ATOM	648	0	ASP			64.495	12.387	24.033	1.00 34.76 A
	ATOM	649	N	ASP			64.498	12.239	26.261	1.00 35.00 A
	ATOM	650	CA	ASP			63.462	13.268	26.369	1.00 36.72 A
	MOTA	651	CB	ASP			63.053	13.465	27.830	1.00 38.27 A
50	MOTA	652	CG	ASP	Α	152	62.237	12.312	28.351	1.00 42.45 A
	ATOM	653	OD1	ASP	Α	152	61.377	11.824	27.579	1.00 43.52 A
	ATOM	654		ASP			62.444	11.900	29.519	1.00 44.28 A
	ATOM	655	c	ASP			63.758	14.627	25.759	1.00 36.47 A
	ATOM	656	o	ASP			62.857	15.289	25.242	1.00 36.12 A
55	MOTA	657	N	GLU			65.021	15.029	25.781	1.00 36.09 A
	MOTA	658	CA	GLU			65.358	16.343	25.292	1.00 35.16 A
	MOTA	659	CB	GLU	Α	153	65.976	17.137	26.442	1.00 39.45 A
	ATOM	660	CG	GLU	Α	153	65.486	16.714	27.830	1.00 45.94 A
	ATOM	661	CD	GLU	А	153	66.383	15.652	28.468	1.00 51.78 A

	MOTA	662		GLU			67.563	15.977	28.746	1.00 54.51 A
	MOTA	663	OE2	GLU	Α	153	65.924	14.500	28.689	1.00 52.47 A
	MOTA	664	C	GLU	Α	153	66.258	16.455	24.073	1.00 32.91 A
	ATOM	665	0	GLU	Α	153	66.304	17.524	23.457	1.00 31.19 A
5	ATOM	666	N	LYS	Α	154	66.959	15.376	23.710	1.00 30.19 A
	MOTA	667	CA	LYS	Α	154	67.898	15.431	22.582	1.00 26.56 A
	ATOM	668	CB	LYS		154	69.323	15.414	23.121	1.00 24.92 A
	ATOM	669	CG	LYS			69.630	16.551	24.041	1.00 23.66 A
	ATOM	670	CD	LYS		154	70.944	16.355	24.750	1.00 20.95 A
10	ATOM	671	CE	LYS		154	71.274	17.583	25.576	1.00 18.98 A
	ATOM	672	NZ	LYS			72.491	17.388	26.360	1.00 19.19 A
	ATOM	673	C	LYS			67.806	14.374	21.487	1.00 25.00 A
	ATOM	674	o	LYS			67.342	13.257	21.701	1.00 25.62 A
	ATOM	675	N	LEU		155	68.276	14.759	20.308	1.00 23.36 A
15	ATOM	676	CA	LEU .			68.337	13.881	19.140	1.00 22.19 A
	ATOM	677	CB	LEU			67.946	14.624	17.864	1.00 21.64 A
	MOTA	678	CG	LEU			66.539	15.167	17.707	1.00 22.58 A
	ATOM	679		LEU .		155	66.437	15.847	16.350	1.00 22.74 A
	ATOM	680		LEU .			65.533	14.034	17.815	1.00 23.23 A
20	MOTA	681	C	LEU .			69.798	13.474	19.004	1.00 20.69 A
	MOTA	682	0	LEU .			70.693	14.287	19.249	1.00 21.61 A
	MOTA	683	N	TYR	Α	156	70.036	12.238	18.592	1.00 18.69 A
	ATOM	684	CA	TYR	Α	156	71.393	11.737	18.431	1.00 18.65 A
	MOTA	685	CB	TYR	Α	156	71.690	10.661	19.489	1.00 18.51 A
25	ATOM	686	CG	TYR	Α	156	71.602	11.148	20.913	1.00 17.86 A
	ATOM	687	CD1	TYR	Α	156	70.372	11.287	21.550	1.00 18.38 A
	ATOM	688	CE1	TYR	А	156	70.286	11.752	22.862	1.00 18.95 A
	ATOM	689	CD2	TYR	А	156	72.755	11.488	21.621	1.00 19.32 A
	ATOM	690	CE2	TYR			72.690	11.957	22.942	1.00 18.14 A
30	ATOM	691	CZ	TYR			71.449	12.086	23.551	1.00 18.56 A
50	ATOM	692	OH	TYR			71.372	12.547	24.838	1.00 18.33 A
	ATOM	693	C	TYR			71.640	11.125	17.059	1.00 18.03 A
	ATOM	694	0	TYR			70.903	10.250	16.646	1.00 18.18 A
	ATOM	695	N	PHE		157	72.662	11.568	16.338	1.00 17.19 A
25										
35	ATOM	696	CA	PHE			72.937	10.934	15.062	1.00 17.15 A
	MOTA	697	CB	PHE			72.980	11.951	13.918	1.00 21.54 A
	MOTA	698	CG	PHE			71.663	12.638	13.651	1.00 26.82 A
	MOTA	699	CD1			157	70.471	12.165	14.221	1.00 30.87 A
	MOTA	700	CD2	PHE			71.617	13.794	12.869	1.00 28.42 A
40	MOTA	701	CE1	PHE			69.249	12.845	14.024	1.00 30.45 A
	MOTA	702	CE2	PHE			70.407	14.483	12.661	1.00 29.44 A
	MOTA	703	CZ	PHE		157	69.224	14.008	13.243	1.00 30.41 A
	ATOM	704	C	PHE			74.286	10.244	15.184	1.00 16.38 A
	MOTA	705	0	PHE			75.256	10.883	15.527	1.00 17.91 A
45	MOTA	706	N	GLY	Α	158	74.347	8.942	14.919	1.00 16.20 A
	ATOM	707	CA	GLY	Α	158	75.614	8.232	15.009	1.00 15.78 A
	ATOM	708	С	GLY	Α	158	76.322	8.285	13.671	1.00 16.51 A
	ATOM	709	0	GLY	Α	158	75.876	7.659	12.710	1.00 17.95 A
	ATOM	710	N	LEU	Α	159	77.423	9.028	13.600	1.00 14.97 A
50	ATOM	711	CA	LEU		159	78.143	9.177	12.342	1.00 15.17 A
	ATOM	712	СВ	LEU			78.264	10.669	12.012	1.00 13.14 A
	ATOM	713	CG	LEU		159	76.989	11.518	12.133	1.00 12.95 A
	ATOM	714		LEU			77.347	13.002	11.872	1.00 7.84 A
	ATOM	715		LEU		159	75.926	11.020	11.138	1.00 7.84 A
55	ATOM	716	CD2	LEU		159	79.535	8.540	12.300	1.00 11.24 A
55							80.136			
	MOTA	717	0	LEU .		159		8.256	13.333	1.00 15.76 A
	MOTA	718	N	SER		160	80.051	8.313	11.097	1.00 14.32 A
	MOTA	719	CA	SER			81.389	7.759	10.984	1.00 14.68 A
	MOTA	720	CB	SER	Α	160	81.699	7.386	9.529	1.00 12.79 A

	MOTA	721	OG	SER			81.395	8.432	8.626	1.00 16.15 A
	ATOM	722	C	SER	Α	160	82.365	8.823	11.509	1.00 15.82 A
	MOTA	723	0	SER	Α	160	82.152	10.029	11.333	1.00 17.75 A
	ATOM	724	N	TYR	Α	161	83.418	8.386	12.184	1.00 16.30 A
5	ATOM	725	CA	TYR	А	161	84.399	9.309	12.740	1.00 17.11 A
	ATOM	726	CB	TYR			84.863	8.785	14.100	1.00 16.09 A
	ATOM	727	CG	TYR			86.020	9.529	14.717	1.00 19.80 A
	ATOM	728		TYR			86.070	10.933	14.700	1.00 18.64 A
1.0	ATOM	729	CE1				87.091	11.625	15.345	1.00 19.50 A
10	MOTA	730	CD2	TYR			87.032	8.837	15.394	1.00 20.09 A
	MOTA	731	CE2	TYR			88.057	9.517	16.047	1.00 21.66 A
	ATOM	732	CZ	TYR			88.085	10.918	16.022	1.00 23.52 A
	MOTA	733	OH	TYR.	Α	161	89.111	11.600	16.674	1.00 22.64 A
	ATOM	734	C	TYR	Α	161	85.594	9.495	11.815	1.00 17.86 A
15	ATOM	735	0	TYR	Α	161	86.269	8.527	11.459	1.00 19.30 A
	ATOM	736	N	ALA	А	162	85.854	10.736	11.418	1.00 18.22 A
	ATOM	737	CA	ALA			86.990	11.040	10.546	1.00 19.59 A
	ATOM	738	CB	ALA			86.569	12.063	9.466	1.00 19.99 A
	ATOM	739	C	ALA			88.051	11.629	11.472	1.00 19.33 A
20		740	0	ALA			88.050	12.828	11.736	1.00 19.11 A
20	ATOM									
	ATOM	741	N	ALA			88.952	10.775	11.956	1.00 18.78 A
	MOTA	742	CA	ALA			89.994	11.165	12.918	1.00 18.84 A
	MOTA	743	CB	ALA .			90.867	9.924	13.279	1.00 19.04 A
	MOTA	744	C	ALA .			90.908	12.357	12.604	1.00 18.22 A
25	ATOM	745	0	ALA	A	163	91.290	13.101	13.508	1.00 16.79 A
	MOTA	746	N	ASN.	Α	164	91.251	12.560	11.340	1.00 17.46 A
	MOTA	747	CA	ASN	Α	164	92.148	13.645	11.023	1.00 17.79 A
	ATOM	748	CB	ASN	Α	164	92.990	13.270	9.803	1.00 20.45 A
	ATOM	749	CG	ASN	А	164	93.919	12.092	10.097	1.00 21.08 A
30	ATOM	750	OD1	ASN	А	164	94.663	12.117	11.066	1.00 21.57 A
	ATOM	751		ASN			93.862	11.059	9.271	1.00 24.54 A
	ATOM	752	C	ASN			91.555	15.044	10.889	1.00 18.34 A
	ATOM	753	o	ASN			92.293	16.005	10.634	1.00 19.83 A
	ATOM	754	N	GLY			90.247	15.176	11.083	1.00 15.01 A
25										
35	ATOM	755	CA	GLY			89.644	16.490	11.022	1.00 15.54 A
	ATOM	756	C	GLY			89.580	17.212	9.683	1.00 17.67 A
	MOTA	757	0	GLY.			89.607	16.600	8.613	1.00 19.49 A
	MOTA	758	N	GLU .			89.510	18.534	9.753	1.00 17.46 A
	MOTA	759	CA	GLU	A	166	89.378	19.379	8.577	1.00 19.26 A
40	MOTA	760	CB	GLU .	Α	166	89.064	20.805	9.019	1.00 21.87 A
	ATOM	761	CG	GLU .	Α	166	88.057	20.917	10.149	1.00 24.70 A
	ATOM	762	CD	GLU	Α	166	87.723	22.359	10.477	1.00 26.05 A
	ATOM	763	OE1	GLU	А	166	88.469	23.251	10.001	1.00 25.93 A
	ATOM	764	OE2				86.726	22.598	11.213	1.00 25.24 A
45	ATOM	765	С	GLU			90.538	19.441	7.592	1.00 20.11 A
	ATOM	766	ō	GLU			91.707	19.501	7.978	1.00 22.88 A
	ATOM	767	N	LEU			90.195	19.443	6.312	1.00 18.72 A
	ATOM	768	CA	LEU			91.173	19.565	5.242	1.00 10.72 A
			CB							
50	MOTA	769		LEU			90.463	19.516	3.888	1.00 15.71 A
50	MOTA	770	CG	LEU			91.238	19.817	2.601	1.00 15.42 A
	MOTA	771		LEU			92.242	18.704	2.343	1.00 14.98 A
	MOTA	772		LEU .			90.265	19.947	1.416	1.00 12.32 A
	MOTA	773	C	LEU			91.817	20.940	5.438	1.00 19.75 A
	MOTA	774	0	LEU			93.030	21.103	5.266	1.00 19.61 A
55	MOTA	775	N	LEU	Α	168	91.001	21.928	5.812	1.00 20.53 A
	ATOM	776	CA	LEU	Α	168	91.516	23.277	6.033	1.00 22.20 A
	ATOM	777	CB	LEU	Α	168	90.436	24.192	6.637	1.00 20.41 A
	ATOM	778	CG	LEU			90.923	25.611	7.024	1.00 21.71 A
	ATOM	779		LEU			91.275	26.413	5.768	1.00 20.09 A

	ATOM	780	CD2	LEU	Α	168	89.837	26.341	7.797	1.00 20.84 A
	ATOM	781	C	LEU	Α	168	92.731	23.245	6.968	1.00 23.07 A
	ATOM	782	0	LEU	Α	168	93.636	24.054	6.838	1.00 22.18 A
	ATOM	783	N	LYS		169	92.742	22.305	7.905	1.00 24.67 A
5	ATOM	784	CA	LYS			93.844	22.192	8.850	1.00 28.56 A
,	ATOM	785	CB	LYS			93.561	21.076	9.858	1.00 20.30 A
		786	CG	LYS		169	94.615	20.933		1.00 31.12 A
	ATOM								10.938	
	MOTA	787	CD	LYS			94.436	19.652	11.765	1.00 39.37 A
	ATOM	788	CE	LYS			94.832	18.410	10.961	1.00 42.26 A
10	MOTA	789	NZ	LYS			94.664	17.131	11.725	1.00 42.83 A
	MOTA	790	C	LYS		169	95.151	21.902	8.119	1.00 29.24 A
	MOTA	791	0	LYS	Α	169	96.190	22.505	8.398	1.00 30.32 A
	MOTA	792	N	TYR	Α	170	95.101	20.970	7.179	1.00 29.12 A
	ATOM	793	CA	TYR	Α	170	96.290	20.619	6.423	1.00 28.18 A
15	MOTA	794	CB	TYR	Α	170	96.037	19.344	5.637	1.00 25.30 A
	MOTA	795	CG	TYR	Α	170	95.926	18.182	6.569	1.00 27.01 A
	ATOM	796	CD1	TYR	А	170	97.072	17.533	7.053	1.00 26.92 A
	ATOM	797	CE1	TYR	А	170	96.974	16.532	8.008	1.00 25.37 A
	ATOM	798	CD2	TYR			94.688	17.792	7.062	1.00 25.14 A
20	ATOM	799	CE2	TYR			94.580	16.807	8.009	1.00 26.49 A
20	ATOM	800	CZ	TYR			95.720	16.179	8.484	1.00 26.98 A
	ATOM	801	OH	TYR			95.580	15.223	9.456	1.00 27.66 A
	MOTA	802	C	TYR			96.690	21.742	5.507	1.00 28.69 A
	MOTA	803	0	TYR			97.875	21.971	5.285	1.00 30.98 A
25	ATOM	804	N	ILE			95.705	22.452	4.976	1.00 28.95 A
	MOTA	805	CA	ILE			96.006	23.550	4.088	1.00 29.79 A
	MOTA	806	CB	ILE			94.721	24.233	3.579	1.00 29.29 A
	MOTA	807		ILE			95.082	25.439	2.714	1.00 28.21 A
	MOTA	808	CG1	ILE	Α	171	93.906	23.227	2.747	1.00 29.66 A
30	ATOM	809	CD1	ILE	Α	171	92.567	23.754	2.224	1.00 29.13 A
	MOTA	810	C	ILE	Α	171	96.897	24.536	4.833	1.00 31.13 A
	MOTA	811	0	ILE	Α	171	97.925	24.956	4.300	1.00 30.93 A
	ATOM	812	N	ARG	А	172	96.525	24.862	6.075	1.00 32.00 A
	ATOM	813	CA	ARG	А	172	97.294	25.789	6.903	1.00 32.60 A
35	ATOM	814	CB	ARG			96.527	26.175	8.163	1.00 32.77 A
-	ATOM	815	CG	ARG			95.257	26.982	7.972	1.00 38.24 A
	ATOM	816	CD	ARG			94.853	27.602	9.335	1.00 43.47 A
	ATOM	817	NE	ARG			93.501	28.181	9.412	1.00 46.65 A
	ATOM	818	CZ	ARG			92.903	28.888	8.448	1.00 47.62 A
40							93.517		7.287	1.00 47.62 A
40	ATOM	819		ARG				29.115		
	MOTA	820		ARG			91.691	29.398	8.659	1.00 45.61 A
	MOTA	821	С	ARG			98.646	25.219	7.338	1.00 32.95 A
	MOTA	822	0	ARG			99.644	25.920	7.311	1.00 34.27 A
	MOTA	823	N	ALA			98.674	23.960	7.761	1.00 32.74 A
45	MOTA	824	CA	ALA			99.912	23.341	8.209	1.00 32.81 A
	MOTA	825	CB	ALA	Α	173	99.668	21.896	8.619	1.00 32.72 A
	MOTA	826	C	ALA	Α	173	101.005	23.400	7.152	1.00 33.67 A
	MOTA	827	0	ALA	Α	173	102.125	23.817	7.438	1.00 33.78 A
	MOTA	828	N	ILE	Α	174	100.698	22.995	5.926	1.00 33.50 A
50	ATOM	829	CA	ILE	Α	174	101.728	23.030	4.896	1.00 33.22 A
	ATOM	830	СВ	ILE			101.731	21.736	4.043	1.00 33.98 A
	ATOM	831		ILE			101.725	20.502	4.950	1.00 32.94 A
	ATOM	832		ILE		174	100.517	21.709	3.125	1.00 33.93 A
	ATOM	833		ILE			100.602	20.631	2.080	1.00 36.79 A
55	ATOM	834	C	ILE			101.638	24.231	3.957	1.00 30.75 A
55	ATOM	835	0	ILE			102.326	24.269	2.938	1.00 32.89 A
		836	N							
	ATOM	835		GLY		175	100.792	25.204	4.287	
	MOTA		CA	GLY			100.671	26.386	3.446	1.00 32.03 A
	MOTA	838	C	GLY	Α	1/5	99.838	26.223	2.184	1.00 32.77 A

	MOTA	839	0	GLY			98.870	26.958	1.976	1.00 35.12 A
	ATOM	840	N	SER	Α	176	100.225	25.291	1.322	1.00 31.63 A
	ATOM	841	CA	SER	Α	176	99.489	25.018	0.091	1.00 31.11 A
	ATOM	842	CB	SER	Α	176	99.810	26.040	-0.996	1.00 31.54 A
5	ATOM	843	OG	SER	А	176	101.141	25.874	-1.464	1.00 33.96 A
	ATOM	844	C			176	99.946	23.640	-0.354	1.00 30.72 A
	ATOM	845	ō			176	100.977	23.154	0.111	1.00 31.29 A
	ATOM	846	N	PHE			99.180	23.018	-1.246	1.00 28.27 A
	ATOM	847	CA	PHE			99.475	21.683	-1.738	1.00 26.27 A
10				PHE						
10	ATOM	848	CB				98.169	20.948	-2.060	
	ATOM	849	CG			177	97.376	20.530	-0.854	1.00 27.90 A
	ATOM	850		PHE			97.551	21.155	0.379	1.00 26.91 A
	MOTA	851	CD2	PHE			96.432	19.503	-0.957	1.00 27.62 A
	ATOM	852	CE1	PHE	Α	177	96.812	20.762	1.477	1.00 26.03 A
15	ATOM	853	CE2	PHE	Α	177	95.684	19.106	0.144	1.00 23.95 A
	ATOM	854	CZ	PHE	Α	177	95.873	19.730	1.357	1.00 25.81 A
	ATOM	855	C	PHE	Α	177	100.299	21.726	-3.008	1.00 26.99 A
	ATOM	856	0	PHE	Α	177	100.115	22.618	-3.832	1.00 27.45 A
	ATOM	857	N	ASP			101.200	20.762	-3.179	1.00 26.09 A
20	ATOM	858	CA	ASP			101.967	20.704	-4.411	1.00 26.09 A
20	ATOM	859	CB	ASP			103.135	19.730	-4.303	1.00 27.73 A
	ATOM	860	CG	ASP			102.689	18.318	-4.023	1.00 27.73 A
		861		ASP			101.601	17.919	-4.510	1.00 37.57 A
	MOTA									
2.5	MOTA	862		ASP			103.431	17.590	-3.324	1.00 35.89 A
25	ATOM	863	С	ASP			100.955	20.202	-5.443	1.00 25.72 A
	MOTA	864	0	ASP			99.763	20.063	-5.128	1.00 24.80 A
	ATOM	865	N	GLU			101.419	19.897	-6.650	1.00 24.80 A
	MOTA	866	CA	GLU			100.514	19.444	-7.697	1.00 25.67 A
	ATOM	867	CB	GLU	Α	179	101.187	19.554	-9.052	1.00 27.44 A
30	ATOM	868	CG	GLU	Α	179	100.197	19.921	-10.129	1.00 31.17 A
	ATOM	869	CD	GLU	Α	179	100.823	19.999	-11.492	1.00 35.24 A
	ATOM	870	OE1	GLU	Α	179	102.016	20.372	-11.572	1.00 35.82 A
	ATOM	871	OE2	GLU	Α	179	100.116	19.707	-12.488	1.00 38.12 A
	ATOM	872	С	GLU	А	179	99.917	18.041	-7.560	1.00 24.90 A
35	ATOM	873	ō	GLU			98.755	17.822	-7.894	1.00 23.01 A
00	ATOM	874	N	THR			100.709	17.095	-7.082	1.00 24.57 A
	ATOM	875	CA	THR			100.709	15.723	-6.923	1.00 24.57 A
	MOTA	876	CB	THR			101.395	14.803	-6.478	1.00 24.65 A
40	MOTA	877		THR			102.525	15.069	-7.304	1.00 25.84 A
40	MOTA	878	CG2				101.021	13.334	-6.624	1.00 23.39 A
	MOTA	879	C	THR			99.110	15.623	-5.902	1.00 25.85 A
	MOTA	880	0	THR			98.149	14.892	-6.111	1.00 25.59 A
	MOTA	881	N	CYS	Α	181	99.237	16.359	-4.799	1.00 25.83 A
	MOTA	882	CA	CYS	Α	181	98.217	16.355	-3.752	1.00 26.26 A
45	ATOM	883	CB	CYS	Α	181	98.778	16.939	-2.451	1.00 27.81 A
	ATOM	884	SG	CYS	Α	181	100.202	16.031	-1.775	1.00 32.72 A
	ATOM	885	C	CYS	Α	181	96.963	17.127	-4.169	1.00 25.20 A
	ATOM	886	0	CYS			95.853	16.696	-3.878	1.00 26.19 A
	ATOM	887	N	THR			97.139	18.262	-4.841	1.00 22.74 A
50	ATOM	888	CA	THR			96.002	19.046	-5.305	1.00 21.82 A
50	ATOM	889	CB	THR			96.453	20.308	-6.103	1.00 21.81 A
	ATOM	890	OG1				97.258	21.161	-5.276	1.00 21.51 A
	ATOM	891	CG2	THR			95.252	21.080	-6.593	1.00 18.62 A
	ATOM	892	C	THR			95.197	18.141	-6.249	1.00 23.45 A
55	MOTA	893	0	THR			93.975	17.997	-6.116	1.00 22.94 A
	ATOM	894	N	ARG			95.897	17.528	-7.202	1.00 22.71 A
	ATOM	895	CA	ARG			95.260	16.648	-8.158	1.00 23.26 A
	ATOM	896	CB	ARG			96.285	16.118	-9.171	1.00 22.46 A
	MOTA	897	CG	ARG	Α	183	95.692	15.140	-10.184	1.00 24.96 A

	MOTA	898	CD	ARG A	183	96.762	14.512	-11.078	1.00 27.09 A
	MOTA	899	NE	ARG A	183	97.372	15.577	-11.849	1.00 33.02 A
	MOTA	900	CZ	ARG A	183	98.637	15.948	-11.732	1.00 33.62 A
	ATOM	901	NH1	ARG A	183	99.440	15.312	-10.885	1.00 32.57 A
5	ATOM	902	NH2	ARG A	183	99.069	17.006	-12.404	1.00 33.25 A
	ATOM	903	С	ARG A	183	94.559	15.475	-7.459	1.00 22.42 A
	ATOM	904	0	ARG A	183	93.393	15.193	-7.721	1.00 21.37 A
	ATOM	905	N	PHE A		95.255	14.800	-6.562	1.00 21.19 A
	ATOM	906	CA	PHE A		94.630	13.673	-5.888	1.00 22.20 A
10	ATOM	907	CB	PHE A		95.615	12.964	-4.966	1.00 23.58 A
	ATOM	908	CG	PHE A		95.029	11.766	-4.283	1.00 25.43 A
	ATOM	909		PHE A		94.916	10.556	-4.954	1.00 25.01 A
	ATOM	910	CD2	PHE A		94.508	11.867	-2.998	1.00 24.35 A
	ATOM	911	CE1	PHE A		94.285	9.460	-4.356	1.00 24.33 A
15	ATOM	912	CE2	PHE A		93.881	10.782	-2.409	1.00 24.71 A
13	ATOM	913	CZ	PHE A		93.771	9.577	-3.094	1.00 24.71 A
	ATOM	914	C	PHE A		93.405	14.074	-5.072	1.00 21.96 A
	MOTA	915	0	PHE A		92.348	13.450	-5.170	1.00 21.31 A
20	MOTA	916	N	TYR A		93.544	15.116	-4.267	1.00 21.18 A
20	MOTA	917	CA	TYR A		92.433	15.543	-3.445	1.00 20.50 A
	MOTA	918	CB	TYR A		92.956	16.425	-2.313	1.00 21.33 A
	MOTA	919	CG	TYR A		93.494	15.550	-1.190	1.00 22.24 A
	ATOM	920		TYR A		92.641	14.670	-0.507	1.00 21.55 A
	MOTA	921	CE1	TYR A		93.127	13.755	0.414	1.00 20.71 A
25	MOTA	922	CD2	TYR A		94.853	15.497	-0.904	1.00 21.37 A
	MOTA	923	CE2	TYR A		95.353	14.579	0.019	1.00 21.80 A
	MOTA	924	CZ	TYR A		94.486	13.705	0.670	1.00 21.18 A
	MOTA	925	OH	TYR A		94.986	12.746	1.519	1.00 19.84 A
	MOTA	926	C	TYR A	185	91.273	16.182	-4.201	1.00 19.27 A
30	MOTA	927	0	TYR A	185	90.112	16.056	-3.801	1.00 17.72 A
	MOTA	928	N	THR A	186	91.576	16.834	-5.314	1.00 17.25 A
	MOTA	929	CA	THR A	186	90.527	17.433	-6.110	1.00 15.61 A
	MOTA	930	CB	THR A	186	91.097	18.366	-7.188	1.00 15.69 A
	MOTA	931	OG1	THR A	186	91.710	19.508	-6.564	1.00 16.11 A
35	ATOM	932	CG2	THR A	186	89.996	18.816	-8.135	1.00 12.68 A
	ATOM	933	С	THR A	186	89.756	16.302	-6.785	1.00 15.75 A
	ATOM	934	0	THR A		88.523	16.350	-6.899	1.00 16.51 A
	ATOM	935	N	ALA A	187	90.478	15.277	-7.218	1.00 14.94 A
	ATOM	936	CA	ALA A	187	89.841	14.136	-7.868	1.00 16.15 A
40	ATOM	937	CB	ALA A		90.905	13.130	-8.382	1.00 13.30 A
	ATOM	938	C	ALA A		88.847	13.450	-6.911	1.00 16.71 A
	ATOM	939	ō	ALA A		87.743	13.075	-7.328	1.00 16.50 A
	ATOM	940	N	GLU A		89.213	13.308	-5.635	1.00 17.10 A
	ATOM	941	CA	GLU A		88.302	12.673	-4.679	1.00 17.85 A
45	ATOM	942	CB	GLU A		88.953	12.514	-3.302	1.00 18.83 A
	ATOM	943	CG	GLU A		90.219	11.665	-3.296	1.00 19.46 A
	ATOM	944	CD	GLU A		90.370	10.795	-2.050	1.00 20.84 A
	ATOM	945		GLU A		90.131	11.276	-0.920	1.00 21.14 A
	ATOM	946		GLU A		90.749	9.616	-2.207	1.00 23.35 A
50	ATOM	947	C	GLU A		87.043	13.516	-4.551	1.00 23.33 A
50	ATOM	948	0	GLU /		85.921	13.005	-4.579	1.00 17.79 A
	ATOM	949	N	ILE A		87.220	14.824	-4.449	1.00 17.09 A
	MOTA	950	CA	ILE A		86.060	15.688	-4.312	1.00 15.61 A
	ATOM	951	CB	ILE A		86.495	17.141	-4.054	1.00 15.83 A
55	ATOM	952		ILE A		85.278	18.019	-3.853	1.00 14.16 A
	MOTA	953		ILE A		87.380	17.199	-2.794	1.00 17.34 A
	MOTA	954		ILE A		87.949	18.583	-2.479	1.00 15.37 A
	MOTA	955	C	ILE A		85.176	15.611	-5.558	1.00 16.00 A
	MOTA	956	0	ILE A	189	83.953	15.530	-5.460	1.00 15.52 A

	ATOM	957	N	VAL	Α	190	85.794	15.619	-6.733	1.00 15.46 A
	MOTA	958	CA	VAL	Α	190	85.031	15.570	-7.964	1.00 15.38 A
	ATOM	959	CB	VAL	Α	190	85.975	15.641	-9.181	1.00 15.37 A
	ATOM	960	CG1	VAL	Α	190	85.273	15.168	-10.447	1.00 14.43 A
5	ATOM	961	CG2	VAL	Α	190	86.454	17.056	-9.350	1.00 14.03 A
	MOTA	962	C	VAL	Α	190	84.228	14.279	-7.987	1.00 17.35 A
	ATOM	963	0	VAL	Α	190	83.016	14.281	-8.258	1.00 15.96 A
	ATOM	964	N	SER	Α	191	84.916	13.182	-7.683	1.00 17.90 A
	ATOM	965	CA	SER	Α	191	84.305	11.858	-7.660	1.00 17.77 A
10	ATOM	966	CB	SER	Α	191	85.377	10.811	-7.344	1.00 18.25 A
	ATOM	967	OG	SER			84.801	9.523	-7.243	1.00 21.13 A
	ATOM	968	C	SER			83,147	11.778	-6.640	1.00 17.28 A
	ATOM	969	ō	SER			82.153	11.095	-6.865	1.00 15.44 A
	ATOM	970	N	ALA			83.291	12.490	-5.525	1.00 17.27 A
15	ATOM	971	CA	ALA			82.267	12.529	-4.485	1.00 15.98 A
	ATOM	972	CB	ALA			82.834	13.164	-3.191	1.00 14.89 A
	ATOM	973	C	ALA			81.078	13.336	-4.988	1.00 16.44 A
	ATOM	974	ō	ALA			79.934	12.922	-4.816	1.00 17.59 A
	ATOM	975	N	LEU			81.340	14.487	-5.609	1.00 16.63 A
20	ATOM	976	CA	LEU			80.253	15.303	-6.140	1.00 16.03 A
20	ATOM	977	CB	LEU			80.769	16.632	-6.688	1.00 16.11 A
	ATOM	978	CG	LEU		193	81.421	17.545	-5.645	1.00 18.83 A
		979		LEU			81.779		-6.276	1.00 18.24 A
	ATOM	980	CD1			193	80.455	18.885 17.751	-4.479	1.00 18.24 A
25	ATOM			LEU			79.509	14.551	-7.236	1.00 18.63 A
23	ATOM	981	C							
	ATOM	982	0	LEU		193	78.286	14.623	-7.325	1.00 18.76 A
	ATOM	983	N	GLU			80.229	13.825	-8.079	1.00 17.87 A
	ATOM	984	CA	GLU		194	79.539	13.082	-9.124	1.00 19.66 A
20	ATOM	985	CB	GLU			80.525	12.295	-9.990	1.00 21.82 A
30	ATOM	986	CG	GLU		194	79.844		-10.947	1.00 21.12 A
	ATOM	987	CD	GLU		194	80.831		-11.758	1.00 25.70 A
	ATOM	988		GLU			81.900	10.122	-11.216	1.00 27.41 A
	MOTA	989	OE2	GLU			80.527		-12.939	1.00 26.12 A
	MOTA	990	С	GLU		194	78.546	12.123	-8.479	1.00 19.58 A
35	ATOM	991	0	GLU			77.420	11.987	-8.937	1.00 17.78 A
	ATOM	992	N	TYR			78.962	11.462	-7.406	1.00 19.09 A
	MOTA	993	CA	TYR			78.063	10.545	-6.736	1.00 19.86 A
	MOTA	994	CB	TYR			78.807	9.740	-5.673	1.00 20.01 A
	MOTA	995	CG	TYR			77.871	8.975	-4.756	1.00 20.45 A
40	MOTA	996		TYR			77.329	7.748	-5.142	1.00 19.40 A
	MOTA	997		TYR			76.471	7.044	-4.296	1.00 18.43 A
	MOTA	998	CD2	TYR			77.527	9.482	-3.500	1.00 20.11 A
	MOTA	999	CE2	TYR			76.678	8.792	-2.652	1.00 19.96 A
	MOTA	1000	CZ	TYR			76.154	7.567	-3.057	1.00 21.07 A
45	MOTA	1001	OH	TYR			75.336	6.859	-2.206	1.00 21.31 A
	MOTA	1002	C	TYR			76.914	11.295	-6.060	1.00 20.00 A
	MOTA	1003	0	TYR			75.775	10.823	-6.033	1.00 21.42 A
	MOTA	1004	N	LEU			77.222	12.455	-5.500	1.00 17.38 A
	MOTA	1005	CA	LEU			76.209	13.226	-4.795	1.00 18.74 A
50	MOTA	1006	CB	LEU		196	76.846	14.412	-4.049	1.00 17.38 A
	MOTA	1007	CG	LEU		196	75.850	15.100	-3.110	1.00 19.04 A
	MOTA	1008		LEU		196	75.423	14.093	-2.061	1.00 17.66 A
	MOTA	1009		LEU		196	76.462	16.338	-2.453	1.00 19.54 A
	MOTA	1010	C	LEU	Α	196	75.148	13.747	-5.751	1.00 18.47 A
55	MOTA	1011	0	LEU	Α	196	73.944	13.608	-5.523	1.00 15.05 A
	MOTA	1012	N	HIS	Α	197	75.622	14.361	-6.824	1.00 18.35 A
	MOTA	1013	CA	HIS	Α	197	74.740	14.915	-7.812	1.00 20.04 A
	MOTA	1014	CB	HIS	Α	197	75.562	15.809	-8.718	1.00 20.29 A
	MOTA	1015	CG	HIS	Α	197	76.048	17.044	-8.025	1.00 21.90 A

	MOTA	1016		HIS			75.766	17.539	-6.794	1.00 19.49 A
	MOTA	1017		HIS			76.892	17.956	-8.621	1.00 20.69 A
	MOTA	1018		HIS			77.104	18.960	-7.789	1.00 20.86 A
	MOTA	1019	NE2	HIS	Α	197	76.433	18.732	-6.676	1.00 19.12 A
5	ATOM	1020	C	HIS	Α	197	73.950	13.858	-8.587	1.00 21.27 A
	MOTA	1021	0	HIS	Α	197	72.865	14.133	-9.099	1.00 21.23 A
	MOTA	1022	N	GLY	А	198	74.487	12.644	-8.644	1.00 21.36 A
	ATOM	1023	CA	GLY			73.810	11.569	-9.339	1.00 20.60 A
	ATOM	1024	С	GLY			72.528	11.203	-8.632	1.00 22.72 A
10	ATOM	1025	ō	GLY			71.593	10.742	-9.269	1.00 22.75 A
	ATOM	1026	N	LYS			72.478	11.411	-7.313	1.00 24.27 A
	ATOM	1027	CA	LYS			71.280	11.105	-6.523	1.00 22.95 A
	ATOM	1028	CB	LYS			71.659	10.629	-5.123	1.00 24.67 A
	ATOM	1029	CG	LYS			72.570	9.429	-5.109	1.00 29.22 A
15	ATOM	1030	CD	LYS			72.986	9.064	-3.701	1.00 23.22 A
13	ATOM	1030	CE	LYS			72.531	7.660	-3.366	1.00 33.11 A
	ATOM	1032	NZ	LYS			72.917	6.686	-4.455	1.00 38.82 A
	MOTA	1033	С	LYS			70.432	12.354	-6.398	1.00 22.39 A
	ATOM	1034	0	LYS			69.558	12.431	-5.542	1.00 22.53 A
20	MOTA	1035	N	GLY			70.710	13.343	-7.241	1.00 21.56 A
	MOTA	1036	CA	GLY			69.953	14.580	-7.203	1.00 22.28 A
	MOTA	1037	C	GLY			70.006	15.326	-5.882	1.00 23.53 A
	MOTA	1038	0	GLY			69.017	15.930	-5.461	1.00 24.83 A
	MOTA	1039	N	ILE			71.161	15.302	-5.225	1.00 22.74 A
25	ATOM	1040	CA	ILE			71.314	15.985	-3.951	1.00 22.95 A
	ATOM	1041	CB	ILE			71.796	15.007	-2.842	1.00 22.51 A
	MOTA	1042		ILE			71.995	15.757	-1.536	1.00 21.73 A
	MOTA	1043	CG1	ILE	Α	201	70.788	13.876	-2.638	1.00 22.48 A
	ATOM	1044	CD1	ILE	Α	201	71.274	12.791	-1.687	1.00 17.26 A
30	ATOM	1045	C	ILE	Α	201	72.361	17.086	-4.076	1.00 24.41 A
	ATOM	1046	0	ILE	Α	201	73.387	16.904	-4.737	1.00 26.41 A
	ATOM	1047	N	ILE			72.118	18.236	-3.470	1.00 23.00 A
	ATOM	1048	CA	ILE			73.137	19.267	-3.520	1.00 24.60 A
	ATOM	1049	CB	ILE			72.729	20.440	-4.420	1.00 26.37 A
35	ATOM	1050		ILE			72.503	19.934	-5.829	1.00 28.52 A
	ATOM	1051		ILE			71.450	21.086	-3.922	1.00 29.04 A
	ATOM	1052		ILE			70.958	22.165	-4.845	1.00 32.55 A
	ATOM	1053	C	ILE			73.482	19.732	-2.105	1.00 24.36 A
	ATOM	1054	ō	ILE			72.605	19.919	-1.257	1.00 25.89 A
40	ATOM	1055	N	HIS			74.776	19.882	-1.856	1.00 22.94 A
40	ATOM	1056	CA	HIS			75.289	20.273	-0.555	1.00 22.34 A
	ATOM	1057	CB	HIS			76.800	20.273	-0.526	1.00 20.00 A
	ATOM	1058	CG	HIS			77.401	20.010	0.840	1.00 20.00 A
		1059		HIS			77.865			1.00 18.43 A
45	ATOM							19.060	1.640	
43	MOTA	1060		HIS			77.569	21.222	1.542	1.00 16.33 A
	MOTA	1061		HIS			78.115	20.953	2.715	1.00 17.77 A
	ATOM	1062		HIS			78.306	19.650	2.800	1.00 18.48 A
	MOTA	1063	С	HIS			74.978	21.731	-0.206	1.00 23.37 A
	MOTA	1064	0	HIS			74.411	22.009	0.860	1.00 22.52 A
50	MOTA	1065	N	ARG			75.361	22.648	-1.101	1.00 23.22 A
	MOTA	1066	CA	ARG			75.126	24.087	-0.934	1.00 23.42 A
	MOTA	1067	CB	ARG			73.674	24.375	-0.544	1.00 22.74 A
	MOTA	1068	CG	ARG			72.663	23.966	-1.561	1.00 24.57 A
	ATOM	1069	CD	ARG	Α	204	71.341	24.681	-1.325	1.00 26.51 A
55	ATOM	1070	NE	ARG	Α	204	70.699	24.299	-0.074	1.00 28.25 A
	MOTA	1071	CZ	ARG	Α	204	69.596	24.871	0.405	1.00 28.63 A
	ATOM	1072	NH1	ARG			69.013	25.849	-0.267	1.00 28.47 A
	ATOM	1073		ARG			69.086	24.472	1.563	1.00 28.55 A
	MOTA	1074	C	ARG			76.017	24.819	0.061	1.00 24.12 A

	ATOM	1075	0	ARG			75.805	26.001	0.308	1.00 26.26 A
	MOTA	1076	N			205	76.990	24.135	0.654	1.00 23.05 A
	MOTA	1077	CA	ASP	Α	205	77.887	24.789	1.595	1.00 20.96 A
	MOTA	1078	CB	ASP	Α	205	77.219	24.883	2.964	1.00 22.31 A
5	ATOM	1079	CG	ASP	Α	205	77.964	25.801	3.914	1.00 26.08 A
	ATOM	1080	OD1	ASP	Α	205	78.812	26.582	3.439	1.00 25.93 A
	ATOM	1081	OD2	ASP	Α	205	77.707	25.751	5.141	1.00 29.89 A
	ATOM	1082	C	ASP			79.210	24.020	1.662	1.00 20.46 A
	ATOM	1083	0	ASP			79.812	23.833	2.716	1.00 21.36 A
10	ATOM	1084	N			206	79.666	23.584	0.504	1.00 18.98 A
	ATOM	1085	CA	LEU			80.893	22.827	0.407	1.00 19.83 A
	ATOM	1086	CB	LEU			80.983	22.229	-0.994	1.00 21.73 A
	ATOM	1087	CG			206	82.039	21.167	-1.298	1.00 24.76 A
	ATOM	1088		LEU		206	81.818	19.943	-0.401	1.00 24.70 A
15	ATOM	1089		LEU		206	81.941	20.789	-2.778	1.00 24.33 A
13	ATOM	1099	CDZ			206	82.093	23.725	0.691	1.00 23.74 A
	ATOM	1091	0			206	82.162	24.857	0.200	
	ATOM	1092	N	LYS		207	83.044	23.226	1.475	1.00 19.79 A
20	ATOM	1093	CA	LYS		207	84.233	24.004	1.821	1.00 19.45 A
20	ATOM	1094	CB	LYS		207	83.825	25.209	2.667	1.00 17.84 A
	MOTA	1095	CG	LYS		207	83.123	24.820	3.933	1.00 19.19 A
	MOTA	1096	CD	LYS		207	82.331	25.969	4.500	1.00 20.50 A
	MOTA	1097	CE			207	81.663	25.556	5.797	1.00 22.10 A
	MOTA	1098	NZ			207	80.955	26.674	6.480	1.00 22.34 A
25	MOTA	1099	C	LYS		207	85.241	23.130	2.565	1.00 19.59 A
	MOTA	1100	0	LYS		207	84.917	22.025	2.985	1.00 20.21 A
	ATOM	1101	N			208	86.480	23.618	2.737	1.00 19.79 A
	MOTA	1102	CD	PRO	Α	208	87.032	24.869	2.188	1.00 18.04 A
	MOTA	1103	CA	PRO	Α	208	87.526	22.853	3.428	1.00 19.22 A
30	MOTA	1104	CB	PRO	Α	208	88.756	23.763	3.297	1.00 19.27 A
	ATOM	1105	CG	PRO	Α	208	88.496	24.521	2.027	1.00 16.27 A
	ATOM	1106	C	PRO	Α	208	87.221	22.477	4.883	1.00 20.50 A
	MOTA	1107	0	PRO	A	208	87.791	21.511	5.411	1.00 21.44 A
	ATOM	1108	N	GLU	Α	209	86.335	23.231	5.530	1.00 20.19 A
35	ATOM	1109	CA	GLU	Α	209	85.956	22.976	6.927	1.00 21.25 A
	ATOM	1110	CB	GLU	А	209	85.383	24.251	7.562	1.00 21.43 A
	ATOM	1111	CG	GLU	А	209	86.330	25.446	7.535	1.00 26.33 A
	ATOM	1112	CD	GLU		209	86.203	26.315	6.270	1.00 30.17 A
	ATOM	1113	OE1	GLU			86.143	25.785	5.131	1.00 30.44 A
40	ATOM	1114		GLU			86.173	27.557	6.422	1.00 33.49 A
	ATOM	1115	С			209	84.920	21.839	7.040	1.00 22.45 A
	ATOM	1116	0			209	84.733	21.255	8.114	1.00 21.98 A
	ATOM	1117	N	ASN			84.269	21.545	5.915	1.00 22.73 A
	ATOM	1118	CA	ASN			83.234	20.514	5.788	1.00 23.66 A
45	ATOM	1119	CB	ASN			82.102	21.013	4.882	1.00 26.67 A
75	ATOM	1120	CG			210	81.104	21.881	5.613	1.00 20.07 A
	ATOM	1121		ASN			80.223	22.481	4.988	1.00 36.52 A
	ATOM	1122		ASN			81.221	21.950	6.946	1.00 34.23 A
	ATOM	1123		ASN			83.775	19.239	5.162	1.00 34.23 A
50			C							
30	ATOM	1124	0	ASN			83.067	18.244	5.081	1.00 21.16 A
	ATOM	1125	N	ILE			85.006	19.293	4.674	1.00 19.42 A
	MOTA	1126	CA	ILE			85.619	18.141	4.029	1.00 17.43 A
	ATOM	1127	CB			211	86.319	18.556	2.708	1.00 14.89 A
	MOTA	1128	CG2	ILE		211	87.046	17.349	2.096	1.00 12.68 A
55	MOTA	1129		ILE			85.277	19.157	1.736	1.00 13.30 A
	MOTA	1130		ILE			85.855	19.805	0.435	1.00 10.47 A
	MOTA	1131	C			211	86.620	17.578	5.024	1.00 17.83 A
	MOTA	1132	0			211	87.685	18.151	5.241	1.00 17.76 A
	ATOM	1133	N	LEU	Α	212	86.265	16.457	5.639	1.00 16.05 A

	MOTA	1134	CA	LEU			87.121	15.871	6.656	1.00 15.84 A
	MOTA	1135	CB	LEU			86.256	15.319	7.793	1.00 14.28 A
	MOTA	1136	CG	LEU			85.108	16.227	8.285	1.00 14.68 A
	MOTA	1137	CD1	LEU	Α	212	84.606	15.715	9.647	1.00 11.38 A
5	MOTA	1138	CD2	LEU	Α	212	85.579	17.685	8.422	1.00 10.88 A
	MOTA	1139	C	LEU	Α	212	88.031	14.787	6.114	1.00 16.77 A
	ATOM	1140	0	LEU	Α	212	87.861	14.335	4.984	1.00 16.78 A
	ATOM	1141	N	LEU			88.999	14.374	6.925	1.00 16.47 A
	ATOM	1142	CA	LEU			89.924	13.332	6.516	1.00 17.64 A
10	ATOM	1143	CB	LEU			91.323	13.926	6.378	1.00 18.08 A
	ATOM	1144	CG	LEU			91.367	14.880	5.176	1.00 17.92 A
	ATOM	1145		LEU			92.076	16.134	5.529	1.00 18.78 A
	ATOM	1146		LEU			92.042	14.187	4.000	1.00 17.07 A
	ATOM	1147	C	LEU			89.919	12.147	7.473	1.00 18.68 A
15	ATOM	1148	ō	LEU			90.091	12.297	8.672	1.00 18.75 A
15	ATOM	1149	N	ASN			89.712	10.955	6.939	1.00 21.19 A
	ATOM	1150	CA	ASN			89.673	9.780	7.797	1.00 23.68 A
		1151		ASN			88.864	8.657	7.122	
	ATOM	1151	CB	ASN			89.613	7.979	6.012	1.00 25.68 A 1.00 31.70 A
20	ATOM									
20	MOTA	1153		ASN			90.680	8.426	5.590	1.00 35.54 A
	ATOM	1154		ASN			89.057	6.886	5.521	1.00 34.56 A
	MOTA	1155	С	ASN			91.077	9.328	8.203	1.00 22.08 A
	ATOM	1156	0	ASN			92.056	9.972	7.864	1.00 20.25 A
	MOTA	1157	N	ALA			91.170	8.239	8.953	1.00 24.03 A
25	MOTA	1158	CA	ALA			92.464	7.738	9.420	1.00 24.26 A
	MOTA	1159	CB	ALA			92.276	6.502	10.277	1.00 21.70 A
	MOTA	1160	C	ALA			93.421	7.426	8.296	1.00 24.90 A
	MOTA	1161	0	ALA			94.615	7.435	8.491	1.00 26.03 A
	MOTA	1162	N	ASP			92.889	7.143	7.108	1.00 25.93 A
30	MOTA	1163	CA	ASP			93.726	6.826	5.963	1.00 26.29 A
	MOTA	1164	CB	ASP	Α	216	93.048	5.773	5.091	1.00 32.31 A
	ATOM	1165	CG	ASP	Α	216	92.862	4.456	5.812	1.00 38.06 A
	MOTA	1166	OD1	ASP	Α	216	93.780	4.043	6.559	1.00 40.03 A
	ATOM	1167	OD2	ASP	Α	216	91.800	3.823	5.616	1.00 42.79 A
35	ATOM	1168	C	ASP	Α	216	94.046	8.026	5.095	1.00 23.69 A
	ATOM	1169	0	ASP	А	216	94.717	7.899	4.085	1.00 24.38 A
	ATOM	1170	N	MET	А	217	93.546	9.187	5.478	1.00 21.45 A
	ATOM	1171	CA	MET			93.752	10.418	4.726	1.00 20.48 A
	ATOM	1172	CB	MET			95.226	10.614	4.396	1.00 21.48 A
40	ATOM	1173	CG	MET			96.081	10.894	5.629	1.00 21.46 A
	ATOM	1174	SD	MET			95.504	12.311	6.580	1.00 25.32 A
	ATOM	1175	CE	MET			96.079	13.722	5.573	1.00 24.08 A
	ATOM	1176	c	MET			92.900	10.556	3.458	1.00 19.63 A
	ATOM	1177	ō	MET			93.245	11.294	2.546	1.00 19.54 A
45	ATOM	1178	N	HIS			91.794	9.824	3.405	1.00 18.82 A
75	ATOM	1179	CA	HIS			90.843	9.945	2.311	1.00 18.81 A
	ATOM	1180	CB	HIS			90.206	8.589	1.994	1.00 20.61 A
	ATOM	1181	CG	HIS			91.097	7.666	1.218	1.00 20.61 A
	ATOM	1182		HIS			91.840	6.605	1.614	
50										
30	MOTA	1183		HIS		218	91.316	7.806	-0.139	1.00 21.30 A
	MOTA	1184		HIS			92.153	6.867	-0.541	1.00 20.75 A
	MOTA	1185		HIS			92.485	6.128	0.501	1.00 20.31 A
	MOTA	1186	C	HIS			89.774	10.925	2.863	1.00 18.97 A
	MOTA	1187	0	HIS		218	89.534	10.965	4.083	1.00 16.48 A
55	MOTA	1188	N	ILE		219	89.166	11.721	1.978	1.00 17.41 A
	MOTA	1189	CA	ILE		219	88.165	12.702	2.387	1.00 16.48 A
	MOTA	1190	CB	ILE		219	87.765	13.695	1.242	1.00 13.43 A
	MOTA	1191	CG2	ILE		219	88.984	14.404	0.698	1.00 10.66 A
	ATOM	1192	CG1	ILE	Α	219	86.973	12.952	0.156	1.00 11.14 A

	ATOM	1193	CD1	ILE .		210	86.505	13.807	-0.995	1.00 4.26 A
	MOTA	1194	C	ILE .			86.875	12.067	2.864	1.00 17.14 A
	MOTA	1195	0	ILE .			86.541	10.943	2.497	1.00 18.77 A
	ATOM	1196	N	GLN .	Α	220	86.159	12.808	3.696	1.00 17.24 A
5	ATOM	1197	CA	GLN .	Α	220	84.878	12.376	4.203	1.00 18.93 A
	ATOM	1198	CB	GLN .	A	220	85.002	11.756	5.604	1.00 22.02 A
	ATOM	1199	CG	GLN .			83.791	10.874	5.952	1.00 26.68 A
	ATOM	1200	CD	GLN .			83.949	10.071	7.253	1.00 31.76 A
				GLN .						
	MOTA	1201					83.437	10.471	8.331	
10	MOTA	1202		GLN .			84.667	8.930	7.161	1.00 29.97 A
	MOTA	1203	C	GLN .			84.077	13.652	4.261	1.00 17.44 A
	ATOM	1204	0	GLN .	Α	220	84.247	14.465	5.170	1.00 17.81 A
	MOTA	1205	N	ILE .	Α	221	83.229	13.852	3.263	1.00 15.69 A
	ATOM	1206	CA	ILE .	Α	221	82.413	15.051	3.230	1.00 16.08 A
15	ATOM	1207	CB	ILE .			81.939	15.359	1.802	1.00 15.82 A
	ATOM	1208		ILE .			80.956	16.519	1.834	1.00 13.95 A
	ATOM	1209		ILE .			83.163	15.627	0.899	1.00 16.66 A
	ATOM	1210		ILE .			82.837	16.045	-0.548	1.00 10.00 A
	MOTA	1211	C	ILE .			81.207	14.892	4.156	1.00 16.52 A
20	MOTA	1212	0	ILE .			80.542	13.860	4.157	1.00 16.03 A
	ATOM	1213	N	THR .	A	222	80.927	15.922	4.948	1.00 17.66 A
	ATOM	1214	CA	THR .	Α	222	79.810	15.862	5.882	1.00 17.70 A
	ATOM	1215	CB	THR .	Α	222	80.331	15.433	7.277	1.00 18.71 A
	ATOM	1216	OG1	THR .	A	222	79.230	15.263	8.172	1.00 16.76 A
25	ATOM	1217	CG2	THR .			81.319	16.470	7.825	1.00 16.79 A
	ATOM	1218	C	THR .			79.069	17.195	5.980	1.00 17.35 A
	ATOM	1219	ō	THR .			79.246	18.062	5.130	1.00 16.83 A
	MOTA	1220	N	ASP.			78.244	17.344	7.018	1.00 18.09 A
	MOTA	1221	CA	ASP .			77.466	18.567	7.268	1.00 19.60 A
30	MOTA	1222	CB	ASP .			78.403	19.778	7.311	1.00 22.73 A
	ATOM	1223	CG	ASP .	A	223	77.763	21.006	7.959	1.00 28.30 A
	ATOM	1224		ASP .			76.565	20.931	8.335	1.00 28.17 A
	ATOM	1225	OD2	ASP .	Α	223	78.480	22.042	8.081	1.00 30.99 A
	ATOM	1226	C	ASP .			76.382	18.799	6.210	1.00 19.52 A
35	ATOM	1227	0	ASP .			76.528	19.655	5.340	1.00 19.39 A
	ATOM	1228	N	PHE .			75.283	18.058	6.303	1.00 18.74 A
	ATOM	1229	CA	PHE .			74.213	18.168	5.321	1.00 18.81 A
	ATOM	1230	CB							1.00 13.81 A
				PHE .			73.825	16.773	4.853	
40	MOTA	1231	CG	PHE .			74.857	16.150	3.971	1.00 17.01 A
40	MOTA	1232		PHE .			74.751	16.250	2.578	1.00 16.10 A
	ATOM	1233		PHE .			75.982	15.543	4.521	1.00 14.00 A
	MOTA	1234	CE1	PHE .	Α	224	75.761	15.752	1.747	1.00 15.92 A
	ATOM	1235	CE2	PHE .	Α	224	77.001	15.042	3.699	1.00 15.63 A
	ATOM	1236	CZ	PHE .	Α	224	76.889	15.147	2.309	1.00 15.79 A
45	ATOM	1237	C	PHE .	Α	224	72.997	18.932	5.775	1.00 19.88 A
	ATOM	1238	0	PHE .			71.961	18.922	5.115	1.00 19.36 A
	ATOM	1239	N	GLY .			73.135	19.599	6.911	1.00 21.38 A
	ATOM	1240	CA	GLY .			72.046	20.388	7.439	1.00 21.30 A
50	MOTA	1241	C	GLY .			71.672	21.545	6.523	1.00 23.43 A
50	MOTA	1242	0	GLY .			70.802	22.323	6.869	1.00 26.22 A
	MOTA	1243	N	THR .			72.311	21.692	5.370	1.00 22.15 A
	ATOM	1244	CA	THR .	A	226	71.930	22.784	4.492	1.00 23.85 A
	ATOM	1245	CB	THR .	Α	226	72.986	23.946	4.465	1.00 24.65 A
	ATOM	1246	OG1	THR .	Α	226	74.197	23.511	3.830	1.00 24.83 A
55	ATOM	1247		THR .			73.285	24.420	5.866	1.00 23.67 A
	ATOM	1248	С	THR .			71.721	22.289	3.073	1.00 24.12 A
	ATOM	1249	Ö	THR .			71.646	23.079	2.129	1.00 22.82 A
	ATOM	1250	N	ALA .			71.620	20.976	2.935	1.00 22.02 A
	ATOM	1251	CA	ALA .	A	221	71.437	20.357	1.637	1.00 26.21 A

	ATOM	1252	CB	ALA			71.774	18.889	1.734	1.00 24.04 A
	MOTA	1253	C	ALA			70.026	20.535	1.064	1.00 28.20 A
	ATOM	1254	0	ALA			69.069	20.767	1.801	1.00 29.29 A
	ATOM	1255	N	ALA			69.912	20.449	-0.258	1.00 28.91 A
5	ATOM	1256	CA	ALA			68.623	20.554	-0.928	1.00 31.02 A
	MOTA	1257	CB	ALA			68.577	21.795	-1.856	1.00 30.45 A
	ATOM	1258	C	ALA			68.501	19.276	-1.745	1.00 32.01 A
	ATOM	1259	0	ALA			69.474	18.846	-2.363	1.00 32.87 A
	ATOM	1260	N	VAL			67.328	18.650	-1.732	1.00 32.95 A
10	MOTA	1261	CA	VAL	Α	229	67.126	17.424	-2.503	1.00 34.26 A
	MOTA	1262	CB	VAL	Α	229	66.468	16.347	-1.657	1.00 33.02 A
	ATOM	1263	CG1	VAL	Α	229	66.194	15.114	-2.498	1.00 33.80 A
	MOTA	1264		VAL			67.356	16.011	-0.496	1.00 31.38 A
	MOTA	1265	C	VAL	Α	229	66.213	17.757	-3.665	1.00 36.36 A
15	MOTA	1266	0	VAL	Α	229	65.065	18.133	-3.455	1.00 38.02 A
	ATOM	1267	N	LEU	Α	230	66.715	17.628	-4.889	1.00 37.75 A
	ATOM	1268	CA	LEU	Α	230	65.917	17.965	-6.066	1.00 39.87 A
	MOTA	1269	CB	LEU	Α	230	66.741	17.775	-7.335	1.00 41.23 A
	MOTA	1270	CG	LEU	Α	230	68.039	18.585	-7.359	1.00 44.16 A
20	MOTA	1271	CD1	LEU	Α	230	68.843	18.208	-8.599	1.00 43.48 A
	ATOM	1272	CD2	LEU	Α	230	67.724	20.087	-7.313	1.00 42.99 A
	ATOM	1273	C	LEU	Α	230	64.646	17.137	-6.162	1.00 40.59 A
	MOTA	1274	0	LEU			64.703	15.954	-6.486	1.00 41.31 A
	MOTA	1275	N	ASN	Α	240	65.964	27.756	-2.248	1.00 83.97 A
25	MOTA	1276	CA	ASN	Α	240	66.331	29.165	-2.370	1.00 84.48 A
	MOTA	1277	CB	ASN			65.294	29.907	-3.225	1.00 85.56 A
	MOTA	1278	CG	ASN			63.949	30.053	-2.524	1.00 86.59 A
	ATOM	1279		ASN			63.850	30.682	-1.465	1.00 87.31 A
	MOTA	1280	ND2	ASN	Α	240	62.904	29.473	-3.115	1.00 86.14 A
30	MOTA	1281	C	ASN			66.433	29.828	-0.994	1.00 83.85 A
	MOTA	1282	0	ASN			66.898	30.963	-0.862	1.00 84.11 A
	ATOM	1283	N	ALA			65.997	29.096	0.023	1.00 83.19 A
	ATOM	1284	CA	ALA			65.996	29.564	1.405	1.00 81.85 A
	MOTA	1285	C	ALA			67.330	29.365	2.127	1.00 79.97 A
35	MOTA	1286	0	ALA			67.349	28.777	3.214	1.00 79.75 A
	MOTA	1287	CB	ALA			64.894	28.825	2.183	1.00 85.17 A
	MOTA	1288	N	PHE			68.433	29.850	1.551	1.00 77.03 A
	MOTA	1289	CA	PHE			69.737	29.680	2.197	1.00 74.85 A
	MOTA	1290	CB	PHE			69.973	28.183	2.438	1.00 73.81 A
40	MOTA	1291	CG	PHE			71.311	27.861	3.015	1.00 72.36 A
	MOTA	1292		PHE			71.595	28.116	4.353	1.00 72.39 A
	MOTA	1293		PHE			72.297	27.312	2.210	1.00 72.03 A
	MOTA	1294		PHE			72.855	27.823	4.879	1.00 72.87 A
4.5	ATOM	1295		PHE			73.553	27.016	2.714	1.00 72.25 A
45	ATOM	1296	CZ	PHE			73.837	27.270	4.054	1.00 72.96 A
	ATOM	1297	С	PHE			70.951	30.283	1.462	1.00 73.13 A
	MOTA	1298	0	PHE			70.958	30.425	0.233	1.00 74.08 A
	MOTA	1299	N	VAL			71.972	30.625	2.250	1.00 69.64 A
50	ATOM	1300	CA	VAL			73.233	31.204	1.777	1.00 65.87 A
50	ATOM	1301	CB	VAL			73.207	32.765	1.834	1.00 66.73 A
	ATOM	1302					74.498	33.344	1.271	1.00 65.65 A
	MOTA	1303	CG2				72.008	33.299	1.084	1.00 66.83 A
	ATOM	1304	C	VAL			74.349	30.708	2.703	1.00 62.21 A
	ATOM	1305	0	VAL			74.471	31.189	3.839	1.00 61.91 A
55	ATOM	1306	N	GLY			75.149	29.760	2.204	1.00 57.62 A
	ATOM	1307	CA	GLY			76.247	29.177	2.967	1.00 51.60 A
	ATOM	1308	C	GLY			77.341	30.132	3.387	1.00 46.47 A
	ATOM	1309	0	GLY			77.063	31.261	3.757	1.00 48.62 A
	MOTA	1310	N	THR	Α	245	78.588	29.686	3.325	1.00 42.06 A

	ATOM	1311	CA	THR			79.709	30.526	3.726	1.00 36.35 A
	MOTA	1312	CB	THR			80.925	29.673	4.096	1.00 35.76 A
	MOTA	1313	OG1	THR	Α	245	80.539	28.740	5.105	1.00 31.66 A
	MOTA	1314	CG2	THR			82.043	30.534	4.651	1.00 33.72 A
5	ATOM	1315	C	THR	Α	245	80.064	31.524	2.637	1.00 34.43 A
	MOTA	1316	0	THR	Α	245	80.309	31.166	1.485	1.00 33.95 A
	MOTA	1317	N	ALA	Α	246	80.087	32.787	3.034	1.00 32.72 A
	ATOM	1318	CA	ALA	А	246	80.338	33.900	2.142	1.00 30.18 A
	ATOM	1319	CB	ALA			80.684	35.127	2.952	1.00 30.18 A
10	ATOM	1320	C	ALA			81.374	33.678	1.062	1.00 29.56 A
	ATOM	1321	o	ALA			81.099	33.895	-0.113	1.00 30.00 A
	ATOM	1322	N	GLN			82.564	33.242	1.445	1.00 28.03 A
	ATOM	1323	CA	GLN			83.623	33.030	0.468	1.00 26.97 A
	ATOM	1324	CB	GLN			84.929	32.706	1.182	1.00 28.32 A
15	ATOM	1325	CG	GLN			85.208	33.659	2.319	1.00 33.33 A
	ATOM	1326	CD	GLN			86.600	33.522	2.863	1.00 36.16 A
	ATOM	1327		GLN			87.556	34.107	2.335	1.00 36.68 A
	ATOM	1328		GLN			86.738	32.731	3.922	1.00 30.00 A
	ATOM	1329	C	GLN			83.355	31.968	-0.583	1.00 35.27 A
20		1330	Ö	GLN			83.962	31.997	-1.653	1.00 25.04 A
20	ATOM									
	ATOM	1331	N	TYR			82.443	31.045	-0.304	1.00 22.51 A
	ATOM	1332	CA	TYR			82.161	29.970	-1.260	1.00 21.98 A
	ATOM	1333	CB	TYR			82.273	28.613	-0.541	1.00 17.74 A
	ATOM	1334	CG	TYR			83.626	28.444	0.117	1.00 14.83 A
25	ATOM	1335		TYR			84.736	28.063	-0.630	1.00 14.53 A
	MOTA	1336		TYR			86.017	28.034	-0.067	1.00 15.65 A
	ATOM	1337		TYR			83.820	28.784	1.460	1.00 13.57 A
	MOTA	1338		TYR			85.086	28.757	2.039	1.00 13.28 A
	MOTA	1339	CZ	TYR			86.192	28.386	1.271	1.00 16.78 A
30	MOTA	1340	OH	TYR			87.471	28.411	1.816	1.00 15.10 A
	MOTA	1341	C	TYR			80.827	30.091	-2.005	1.00 22.23 A
	ATOM	1342	0	TYR	Α	248	80.523	29.268	-2.866	1.00 22.78 A
	MOTA	1343	N	VAL	Α	249	80.054	31.126	-1.680	1.00 21.81 A
	MOTA	1344	CA	VAL	Α	249	78.760	31.395	-2.308	1.00 22.22 A
35	ATOM	1345	CB	VAL	Α	249	78.077	32.634	-1.640	1.00 22.82 A
	ATOM	1346	CG1	VAL	Α	249	76.904	33.139	-2.496	1.00 22.57 A
	ATOM	1347	CG2	VAL	Α	249	77.606	32.270	-0.243	1.00 22.62 A
	ATOM	1348	С	VAL	Α	249	78.878	31.666	-3.818	1.00 21.92 A
	ATOM	1349	0	VAL	Α	249	79.733	32.428	-4.255	1.00 20.01 A
40	ATOM	1350	N	SER	Α	250	78.012	31.045	-4.609	1.00 22.88 A
	ATOM	1351	CA	SER	Α	250	78.030	31.259	-6.049	1.00 24.81 A
	ATOM	1352	CB	SER	А	250	77.357	30.105	-6.792	1.00 25.82 A
	ATOM	1353	OG	SER	А	250	75.999	29.984	-6.419	1.00 27.07 A
	ATOM	1354	С	SER			77.288	32.546	-6.357	1.00 26.22 A
45	ATOM	1355	0	SER			76.438	33.004	-5.582	1.00 25.88 A
	ATOM	1356	N	PRO			77.592	33.148	-7.506	1.00 26.70 A
	ATOM	1357	CD	PRO			78.632	32.813	-8.495	1.00 27.24 A
	ATOM	1358	CA	PRO			76.908	34.393	-7.847	1.00 27.08 A
	ATOM	1359	CB	PRO			77.637	34.860	-9.113	1.00 25.51 A
50	ATOM	1360	CG	PRO			78.171	33.590	-9.701	1.00 27.43 A
50	ATOM	1361	C	PRO			75.399	34.288	-8.026	1.00 28.00 A
	ATOM	1362	Ö	PRO			74.684	35.218	-7.678	1.00 28.30 A
		1363	N	GLU			74.908	33.166	-8.550	1.00 28.81 A
	ATOM									
	ATOM	1364	CA	GLU			73.469	33.012	-8.768	1.00 29.67 A
55	ATOM	1365	CB	GLU			73.151	31.684	-9.463	1.00 29.72 A
	MOTA	1366	CG	GLU			73.698	30.453	-8.740	1.00 31.04 A
	ATOM	1367	CD	GLU			75.106	30.075	-9.191	1.00 30.61 A
	ATOM	1368		GLU			75.880	30.973	-9.597	1.00 30.55 A
	ATOM	1369	OE2	GLU	Α	252	75.434	28.872	-9.130	1.00 30.80 A

	MOTA	1370	Ç	GLU			72.709	33.083	-7.462	1.00 30.83 A
	MOTA	1371	0	GLU			71.563	33.530	-7.423	1.00 31.87 A
	MOTA	1372	N	LEU	Α	253	73.351	32.639	-6.388	1.00 32.71 A
	MOTA	1373	CA	LEU	Α	253	72.734	32.655	-5.073	1.00 33.94 A
5	ATOM	1374	CB	LEU	Α	253	73.612	31.901	-4.081	1.00 37.40 A
	MOTA	1375	CG	LEU	Α	253	72.967	31.086	-2.950	1.00 41.64 A
	ATOM	1376	CD1	LEU	Α	253	72.067	31.925	-2.048	1.00 43.86 A
	ATOM	1377	CD2	LEU	Α	253	72.144	30.017	-3.597	1.00 45.52 A
	ATOM	1378	С	LEU			72.545	34.095	-4.603	1.00 35.67 A
10	ATOM	1379	o	LEU			71.589	34.392	-3.897	1.00 37.48 A
	ATOM	1380	N	LEU			73.451	34.989	-4.995	1.00 36.38 A
	ATOM	1381	CA	LEU			73.372	36.397	-4.600	1.00 36.66 A
	ATOM	1382	CB	LEU			74.764	37.032	-4.572	1.00 33.81 A
	ATOM	1383	CG	LEU			75.824	36.402	-3.674	1.00 33.40 A
15	ATOM	1384		LEU			77.183	37.022	-3.982	1.00 30.48 A
15	ATOM	1385		LEU			75.440	36.574	-2.208	1.00 30.40 A
	ATOM	1386	C	LEU			72.485	37.240	-5.511	1.00 31.43 A
	ATOM			LEU			72.079	38.328	-5.133	1.00 38.85 A
		1387 1388	0	THR			72.079	36.754	-6.709	1.00 38.85 A
20	ATOM		N							
20	ATOM	1389	CA	THR			71.358	37.528	-7.624	1.00 47.21 A
	ATOM	1390	CB	THR			72.102	37.847	-8.941	1.00 47.08 A
	MOTA	1391		THR			72.008	36.718	-9.814	1.00 48.56 A
	MOTA	1392		THR			73.581	38.157	-8.686	1.00 45.65 A
	MOTA	1393	С	THR			70.044	36.848	-8.009	1.00 51.00 A
25	MOTA	1394	0	THR			69.348	37.323	-8.903	1.00 51.80 A
	MOTA	1395	N	GLU			69.696	35.745	-7.353	1.00 55.01 A
	ATOM	1396	CA	GLU			68.450	35.044	-7.683	1.00 58.97 A
	MOTA	1397	CB	GLU			68.679	34.057	-8.832	1.00 59.81 A
	MOTA	1398	CG	GLU	Α	256	68.922	34.707	-10.181	1.00 63.59 A
30	MOTA	1399	CD	GLU			69.343	33.707	-11.240	1.00 65.64 A
	ATOM	1400	OE1	GLU	Α	256	68.727	32.617	-11.310	1.00 67.44 A
	ATOM	1401	OE2	GLU	Α	256	70.285	34.015	-12.007	1.00 66.61 A
	ATOM	1402	C	GLU	Α	256	67.859	34.279	-6.512	1.00 60.83 A
	ATOM	1403	0	GLU	Α	256	66.701	33.861	-6.563	1.00 61.27 A
35	ATOM	1404	N	ALA	Α	257	68.657	34.100	-5.463	1.00 62.31 A
	ATOM	1405	CA	ALA	А	257	68.234	33.348	-4.285	1.00 63.29 A
	ATOM	1406	CB	ALA	А	257	66.867	33.847	-3.784	1.00 62.76 A
	ATOM	1407	С	ALA			68.157	31.860	-4.651	1.00 63.64 A
	ATOM	1408	0	ALA			67.790	31.028	-3.825	1.00 64.96 A
40	ATOM	1409	N	SER			68.523	31.532	-5.888	1.00 62.79 A
	ATOM	1410	CA	SER			68.485	30.150	-6.378	1.00 62.30 A
	ATOM	1411	СВ	SER			68.049	30.144	-7.847	1.00 63.00 A
	ATOM	1412	OG	SER			68.762	31.129	-8.582	1.00 63.40 A
	ATOM	1413	c	SER			69.816	29.402	-6.237	1.00 61.09 A
45	ATOM	1414	ō	SER			70.862	30.009	-6.009	1.00 62.12 A
75	ATOM	1415	N	ALA			69.774	28.083	-6.389	1.00 58.47 A
	ATOM	1416	CA	ALA			70.979	27.270	-6.278	1.00 55.79 A
	ATOM	1417	CB	ALA			71.403	27.164	-4.837	1.00 56.24 A
	ATOM	1417		ALA			70.738	25.886	-6.842	
50			C							
30	ATOM	1419	0	ALA			69.641	25.347	-6.736	1.00 54.10 A
	ATOM	1420	N	CYS			71.768	25.302	-7.433	1.00 49.75 A
	ATOM	1421	CA	CYS			71.623	23.988	-8.015	1.00 45.68 A
	ATOM	1422	CB	CYS			71.067	24.106	-9.438	1.00 48.50 A
	MOTA	1423	SG	CYS			69.936	22.732	-9.899	1.00 57.53 A
55	MOTA	1424	С	CYS			72.980	23.318	-8.022	1.00 41.30 A
	MOTA	1425	0	CYS			73.892	23.762	-7.335	1.00 39.24 A
	MOTA	1426	N	LYS			73.118	22.258	-8.805	1.00 36.63 A
	MOTA	1427	CA	LYS			74.369	21.535	-8.866	1.00 33.81 A
	MOTA	1428	CB	LYS	Α	261	74.261	20.416	-9.897	1.00 34.27 A

	MOTA	1429	CG	LYS			73.250	19.362	-9.488	1.00 34.04 A
	MOTA	1430	CD	LYS			72.995		-10.577	1.00 33.10 A
	MOTA	1431	CE	LYS			71.983		-10.105	1.00 32.48 A
	MOTA	1432	NZ	LYS	Α	261	71.660	16.357	-11.176	1.00 33.10 A
5	ATOM	1433	C	LYS	Α	261	75.565	22.419	-9.153	1.00 31.80 A
	MOTA	1434	0	LYS	Α	261	76.636	22.214	-8.589	1.00 31.89 A
	ATOM	1435	N	SER	Α	262	75.389	23.405	-10.025	1.00 29.92 A
	ATOM	1436	CA	SER	Α	262	76.477	24.314	-10.354	1.00 28.19 A
	MOTA	1437	CB	SER	Α	262	76.034	25.309	-11.417	1.00 29.90 A
10	MOTA	1438	OG	SER	Α	262	76.184	24.732	-12.695	1.00 34.45 A
	MOTA	1439	C	SER	Α	262	77.047	25.069	-9.155	1.00 25.77 A
	ATOM	1440	0	SER			78.225	25.405	-9.146	1.00 26.59 A
	MOTA	1441	N	SER	Α	263	76.216	25.347	-8.159	1.00 23.42 A
	ATOM	1442	CA			263	76.663	26.040	-6.953	1.00 23.04 A
15	ATOM	1443	CB			263	75.502	26.209	-5.979	1.00 24.64 A
	ATOM	1444	OG			263	74.463	26.963	-6.572	1.00 31.12 A
	ATOM	1445	C			263	77.777	25.233	-6.283	1.00 21.37 A
	ATOM	1446	ō	SER			78.745	25.803	-5.788	1.00 20.74 A
	ATOM	1447	N	ASP			77.640	23.909	-6.268	1.00 19.11 A
20	ATOM	1448	CA	ASP			78.674	23.062	-5.682	1.00 19.35 A
20	ATOM	1449	CB	ASP			78.206	21.609	-5.579	1.00 18.45 A
	ATOM	1450	CG	ASP			77.164	21.406	-4.500	1.00 19.39 A
	ATOM	1451		ASP			76.998	22.304	-3.649	1.00 20.34 A
	ATOM	1452		ASP			76.522	20.338	-4.488	1.00 19.48 A
25	ATOM	1453	C	ASP			79.943	23.127	-6.542	1.00 19.40 A
23	ATOM	1454	ŏ	ASP			81.052	23.147	-6.018	1.00 20.70 A
	ATOM	1455	N	LEU			79.772	23.162	-7.864	1.00 20.70 A
	ATOM	1456	CA	LEU			80.898	23.232	-8.774	1.00 17.00 A
	ATOM	1457	CB	LEU			80.406		-10.208	1.00 17.42 A
30	ATOM	1458	CG	LEU			79.683		-10.208	1.00 19.58 A
30		1459							-11.879	
	ATOM			LEU			79.189			1.00 17.18 A
	ATOM	1460		LEU			80.625		-10.168	1.00 14.91 A
	ATOM	1461	C	LEU			81.619	24.566	-8.600	1.00 19.06 A
25	ATOM	1462		LEU			82.850	24.649	-8.697	1.00 18.60 A
35	ATOM	1463	N	TRP			80.853	25.621	-8.350	1.00 18.60 A
	ATOM	1464	CA	TRP			81.468	26.902	-8.107	1.00 18.62 A
	ATOM	1465	CB	TRP			80.405	27.976	-7.876	1.00 19.75 A
	ATOM	1466	CG			266	80.997	29.277	-7.382	1.00 21.53 A
40	ATOM	1467		TRP			81.357	30.420	-8.174	1.00 22.40 A
40	ATOM	1468	CE2	TRP			81.917	31.375	-7.296	1.00 22.70 A
	ATOM	1469		TRP			81.260	30.728	-9.541	1.00 21.62 A
	ATOM	1470		TRP			81.344	29.582	-6.094	1.00 20.15 A
	MOTA	1471		TRP			81.896	30.835	-6.037	1.00 20.80 A
4.5	ATOM	1472	CZ2				82.382	32.624	-7.739	1.00 22.47 A
45	ATOM	1473		TRP			81.721	31.961	-9.981	1.00 22.48 A
	ATOM	1474	CH2	TRP			82.276	32.898	-9.080	1.00 23.40 A
	MOTA	1475	C	TRP			82.338	26.734	-6.857	1.00 18.89 A
	MOTA	1476	0	TRP			83.523	27.070	-6.875	1.00 20.01 A
	MOTA	1477	N	ALA			81.755	26.204	-5.780	1.00 16.09 A
50	MOTA	1478	CA	ALA			82.502	25.994	-4.540	1.00 15.55 A
	MOTA	1479	CB	ALA			81.630	25.313	-3.499	1.00 13.20 A
	MOTA	1480	C	ALA			83.738	25.145	-4.813	1.00 16.44 A
	MOTA	1481	0	ALA			84.802	25.345	-4.218	1.00 17.65 A
	MOTA	1482	N	LEU			83.597	24.181	-5.710	1.00 15.96 A
55	MOTA	1483	CA	LEU			84.732	23.336	-6.055	1.00 17.56 A
	MOTA	1484	CB	LEU			84.315	22.281	-7.098	1.00 16.91 A
	MOTA	1485	CG	LEU	Α	268	85.477	21.535	-7.775	1.00 16.43 A
	MOTA	1486		LEU			86.214	20.697	-6.766	1.00 15.17 A
	MOTA	1487	CD2	LEU	Α	268	84.947	20.643	-8.871	1.00 17.18 A

	MOTA	1488	C	LEU .	A 2	68	85.892	24.193	-6.599	1.00	15.96 A
	ATOM	1489	0	LEU .	A 2	68	87.032	24.040	-6.178	1.00	14.54 A
	ATOM	1490	N	GLY .	A 2	69	85.578	25.092	-7.530	1.00	17.15 A
	ATOM	1491	CA	GLY .			86.590	25.957	-8.116		18.32 A
5		1492	C	GLY .			87.339	26.722	-7.042		19.39 A
	ATOM	1493	ō	GLY .			88.579	26.777	-7.042		19.66 A
	ATOM	1494	N	CYS .			86.579	27.297	-6.111		17.50 A
	ATOM	1495	CA	CYS .			87.154	28.043	-5.010		17.72 A
	ATOM	1496	CB	CYS .			86.047	28.551	-4.088		18.96 A
10		1496	SG	CYS .			84.981	29.801	-4.798		19.62 A
10											
	ATOM	1498	C	CYS .			88.114	27.182	-4.201		18.63 A
	ATOM	1499	0	CYS .			89.213	27.612	-3.850		18.78 A
	ATOM	1500	N				87.679	25.962	-3.900		20.05 A
1.5	ATOM	1501	CA	ILE .			88.479	25.019	-3.130		20.08 A
15		1502	CB	ILE .			87.668	23.755	-2.812		20.09 A
	ATOM	1503		ILE .			88.592	22.654	-2.302		18.31 A
	MOTA	1504		ILE .			86.558	24.104	-1.810		18.38 A
	MOTA	1505		ILE .			85.396	23.125	-1.783		14.68 A
	MOTA	1506	C	ILE .			89.761	24.629	-3.858		20.41 A
20		1507	0	ILE .			90.826	24.548	-3.234		21.81 A
	MOTA	1508	N	ILE .			89.669	24.398	-5.166		18.41 A
	ATOM	1509	CA	ILE .			90.860	24.035	-5.934		19.20 A
	MOTA	1510	CB	ILE .			90.526	23.730	-7.412		20.04 A
	MOTA	1511		ILE .			91.808	23.488	-8.199		17.73 A
25	MOTA	1512	CG1	ILE .	A 2	72	89.602	22.523	-7.513	1.00	19.47 A
	MOTA	1513	CD1	ILE .	A 2	72	89.001	22.386	-8.872	1.00	20.31 A
	ATOM	1514	C	ILE .	A 2	72	91.858	25.191	-5.932	1.00	19.57 A
	ATOM	1515	0	ILE .	A 2	72	93.061	24.978	-5.884	1.00	20.97 A
	ATOM	1516	N	TYR .	A 2	73	91.338	26.413	-6.028	1.00	19.42 A
30	ATOM	1517	CA	TYR .	A 2	73	92.157	27.606	-6.041	1.00	18.41 A
	ATOM	1518	CB	TYR .	A 2	73	91.272	28.826	-6.294	1.00	18.70 A
	ATOM	1519	CG	TYR .			91.998	30.147	-6.252		19.81 A
	ATOM	1520		TYR .			92.357	30.729	-5.035		21.25 A
	ATOM	1521		TYR .			93.072	31.936	-4.990		22.12 A
35		1522	CD2	TYR .			92.366	30.804	-7.433		20.45 A
	ATOM	1523	CE2	TYR .			93.081	32.005	-7.403		20.42 A
	ATOM	1524	CZ	TYR .			93.432	32.563	-6.178		23.33 A
	ATOM	1525	OH	TYR .			94.159	33.731	-6.138		23.26 A
	ATOM	1526	C	TYR .			92.848	27.699	-4.687		19.40 A
40		1527	ō	TYR .			94.051	27.945	-4.598		19.44 A
	ATOM	1528	N	GLN .			92.079	27.471	-3.632		19.53 A
	ATOM	1529	CA	GLN .			92.602	27.517	-2.278		21.26 A
	ATOM	1530	CB	GLN .			91.450	27.399	-1.290		22.36 A
	ATOM	1531	CG	GLN .			91.838	27.629	0.142		21.87 A
45		1532	CD	GLN .			90.643	27.531	1.054		23.64 A
73	ATOM	1533		GLN .			89.499	27.479	0.585		22.12 A
	ATOM	1534		GLN .			90.890	27.517	2.369		24.45 A
	ATOM	1535	C	GLN .			93.656	26.435	-1.980		22.20 A
	ATOM	1536	0	GLN .			94.549	26.652	-1.160		22.20 A
50											
30		1537	N	LEU .			93.558	25.275	-2.625		21.82 A
	ATOM	1538	CA	LEU .			94.550	24.223	-2.385		21.95 A
	MOTA	1539	CB	LEU .			94.104	22.886	-3.015		19.19 A
	ATOM	1540	CG	LEU .			92.934	22.153	-2.341		19.86 A
	ATOM	1541		LEU .		75	92.528	20.915	-3.134		19.79 A
55		1542		LEU .			93.333	21.757	-0.938		16.56 A
	MOTA	1543	C	LEU .			95.910	24.630	-2.962		21.62 A
	MOTA	1544	0	LEU .			96.950	24.414	-2.353		21.98 A
	MOTA	1545	N	VAL .			95.884	25.239	-4.137		20.54 A
	MOTA	1546	CA	VAL .	A 2	76	97.095	25.639	-4.828	1.00	21.48 A

	ATOM	1547	CB	VAL			96.810	25.795	-6.338	1.00 21.76 A
	ATOM	1548		VAL			98.035	26.269	-7.061	1.00 20.72 A
	MOTA	1549	CG2	VAL	Α	276	96.332	24.479	-6.908	1.00 21.98 A
	ATOM	1550	C	VAL	Α	276	97.696	26.946	-4.315	1.00 23.17 A
5	ATOM	1551	0	VAL	Α	276	98.913	27.055	-4.141	1.00 24.82 A
	ATOM	1552	N	ALA	Α	277	96.837	27.934	-4.085	1.00 22.20 A
	ATOM	1553	CA	ALA	А	277	97.271	29.230	-3.628	1.00 19.31 A
	ATOM	1554	CB	ALA			96.339	30.293	-4.174	1.00 19.24 A
	ATOM	1555	C	ALA			97.380	29.350	-2.113	1.00 20.10 A
10	ATOM	1556	o	ALA			98.096	30.222	-1.622	1.00 20.73 A
	ATOM	1557	N	GLY			96.686	28.493	-1.368	1.00 19.16 A
	ATOM	1558	CA	GLY			96.748	28.579	0.084	1.00 18.62 A
	ATOM	1559	C	GLY			95.634	29.425	0.677	1.00 21.09 A
	ATOM	1560	ō	GLY			95.462	29.483	1.903	1.00 20.36 A
15	ATOM	1561	N	LEU			94.865	30.084	-0.190	1.00 20.50 A
13	ATOM	1562	CA	LEU			93.742	30.004	0.254	1.00 24.03 A
	ATOM	1563	CB	LEU			94.190	32.365	0.448	1.00 23.98 A
	MOTA	1564	CG	LEU			95.322	32.744	1.396	1.00 25.93 A
20	ATOM	1565		LEU			95.622	34.215	1.140	1.00 25.95 A
20	MOTA	1566		LEU			94.950	32.511	2.873	1.00 24.23 A
	MOTA	1567	C	LEU			92.575	30.940	-0.735	1.00 23.96 A
	MOTA	1568	0	LEU			92.759	30.776	-1.939	1.00 23.93 A
	MOTA	1569	N	PRO			91.353	31.151	-0.231	1.00 24.60 A
	ATOM	1570	CD	PRO			90.987	31.360	1.185	1.00 23.93 A
25	ATOM	1571	CA	PRO			90.177	31.208	-1.109	1.00 24.56 A
	MOTA	1572	CB	PRO			89.024	31.319	-0.116	1.00 24.33 A
	ATOM	1573	CG	PRO			89.656	32.027	1.076	1.00 24.23 A
	MOTA	1574	C	PRO	Α	280	90.324	32.453	-2.033	1.00 25.82 A
	ATOM	1575	0	PRO	Α	280	90.892	33.458	-1.632	1.00 27.28 A
30	ATOM	1576	N	PRO	Α	281	89.798	32.396	-3.268	1.00 25.40 A
	ATOM	1577	CD	PRO	Α	281	88.807	31.385	-3.660	1.00 26.04 A
	ATOM	1578	CA	PRO	Α	281	89.862	33.470	-4.272	1.00 24.99 A
	ATOM	1579	CB	PRO	Α	281	89.150	32.871	-5.489	1.00 24.76 A
	ATOM	1580	CG	PRO	Α	281	88.882	31.442	-5.137	1.00 26.48 A
35	ATOM	1581	C	PRO			89.254	34.836	-3.921	1.00 25.24 A
	ATOM	1582	o	PRO			89.803	35.886	-4.272	1.00 25.07 A
	ATOM	1583	N	PHE			88.103	34.821	-3.264	1.00 24.47 A
	ATOM	1584	CA	PHE			87.435	36.059	-2.918	1.00 24.29 A
	ATOM	1585	CB	PHE			85.964	35.961	-3.320	1.00 23.11 A
40	ATOM	1586	CG	PHE			85.759	35.596	-4.774	1.00 21.99 A
	ATOM	1587		PHE			85.936	36.543	-5.775	1.00 20.97 A
	ATOM	1588		PHE			85.448	34.285	-5.139	1.00 21.76 A
	ATOM	1589		PHE			85.812	36.194	-7.124	1.00 20.59 A
	ATOM	1590		PHE			85.325	33.923	-6.469	1.00 20.98 A
45	ATOM	1591	CZ	PHE			85.509	34.885	-7.471	1.00 20.90 A
43			C				87.579			1.00 25.85 A
	ATOM	1592		PHE				36.366	-1.435	
	ATOM	1593	0	PHE			86.963	35.707	-0.596	1.00 27.04 A
	ATOM	1594	N	ARG			88.414	37.358	-1.124	1.00 27.56 A
	MOTA	1595	CA	ARG			88.676	37.784	0.260	1.00 27.41 A
50	MOTA	1596	CB	ARG			90.116	37.451	0.648	1.00 28.05 A
	ATOM	1597	CG	ARG			90.523	36.020	0.327	1.00 32.73 A
	MOTA	1598	CD	ARG			91.944	35.722	0.788	1.00 36.54 A
	ATOM	1599	NE	ARG			92.942	36.490	0.043	1.00 39.92 A
	MOTA	1600	CZ	ARG			93.202	36.329	-1.253	1.00 42.59 A
55	MOTA	1601		ARG			92.544	35.421	-1.961	1.00 44.54 A
	ATOM	1602		ARG			94.112	37.090	-1.853	1.00 43.94 A
	ATOM	1603	C	ARG			88.445	39.291	0.394	1.00 27.01 A
	ATOM	1604	0	ARG			88.682	40.047	-0.557	1.00 26.54 A
	ATOM	1605	N	ALA	Α	284	87.977	39.724	1.568	1.00 26.05 A

	ATOM	1606	CA	ALA			87.694	41.135	1.812	1.00 23.42 A
	MOTA	1607	CB	ALA	Α	284	86.529	41.579	0.967	1.00 21.82 A
	MOTA	1608	C	ALA	Α	284	87.386	41.383	3.280	1.00 24.72 A
	MOTA	1609	0	ALA	Α	284	87.193	40.440	4.048	1.00 24.83 A
5	ATOM	1610	N	GLY	Α	285	87.330	42.663	3.659	1.00 25.04 A
	ATOM	1611	CA	GLY	А	285	87.055	43.039	5.035	1.00 23.67 A
	ATOM	1612	C	GLY			85.761	42.542	5.652	1.00 25.13 A
	ATOM	1613	ō	GLY			85.718	42.302	6.855	1.00 26.60 A
	ATOM	1614	N	ASN			84.700	42.399	4.862	1.00 24.84 A
10	ATOM	1615	CA	ASN			83.418	41.923	5.391	1.00 23.82 A
	ATOM	1616	CB	ASN			82.567	43.098	5.899	1.00 23.66 A
	ATOM	1617	CG	ASN			82.362	44.190	4.843	1.00 24.14 A
	ATOM	1618		ASN			81.835	43.947	3.747	1.00 24.14 A
	ATOM	1619		ASN			82.776	45.402	5.178	1.00 22.27 A
1.5										
15	MOTA	1620	С	ASN			82.672	41.185	4.296	1.00 24.75 A
	MOTA	1621	0	ASN			83.124	41.160	3.153	1.00 25.32 A
	MOTA	1622	N	GLU			81.522	40.610	4.630	1.00 26.04 A
	MOTA	1623	CA	GLU			80.746	39.865	3.641	1.00 27.47 A
	ATOM	1624	CB	GLU			79.549	39.175	4.287	1.00 30.33 A
20	MOTA	1625	CG	GLU			79.935	38.202	5.364	1.00 36.51 A
	ATOM	1626	CD	GLU			78.792	37.288	5.766	1.00 41.45 A
	MOTA	1627	OE1	GLU	Α	287	77.608	37.712	5.641	1.00 43.02 A
	ATOM	1628	OE2	GLU	Α	287	79.092	36.155	6.222	1.00 41.33 A
	MOTA	1629	C	GLU	Α	287	80.250	40.679	2.467	1.00 25.95 A
25	ATOM	1630	0	GLU	Α	287	80.279	40.203	1.330	1.00 25.67 A
	ATOM	1631	N	TYR	Α	288	79.772	41.893	2.730	1.00 25.20 A
	ATOM	1632	CA	TYR	Α	288	79.276	42.731	1.644	1.00 22.91 A
	ATOM	1633	CB	TYR	А	288	78.870	44.113	2.152	1.00 22.98 A
	ATOM	1634	CG	TYR	А	288	78.459	45.068	1.038	1.00 23.01 A
30	ATOM	1635		TYR			77.166	45.031	0.478	1.00 24.16 A
	ATOM	1636		TYR			76.814	45.869	-0.589	1.00 22.73 A
	ATOM	1637	CD2				79.376	45.965	0.508	1.00 21.34 A
	ATOM	1638	CE2	TYR			79.043	46.796	-0.551	1.00 23.71 A
	ATOM	1639	CZ	TYR			77.771	46.748	-1.099	1.00 25.48 A
35	ATOM	1640	OH	TYR			77.490	47.571	-2.172	1.00 26.98 A
33	ATOM	1641	C	TYR			80.352	42.882	0.578	1.00 26.36 A
			0							
	ATOM	1642		TYR			80.068	42.735	-0.603	1.00 22.65 A
	MOTA	1643	N	LEU			81.590	43.155	0.993	1.00 22.04 A
40	ATOM	1644	CA	LEU			82.691	43.326	0.037	1.00 23.92 A
40	MOTA	1645	CB	LEU			83.927	43.907	0.748	1.00 21.71 A
	MOTA	1646	CG	LEU			83.661	45.326	1.298	1.00 23.89 A
	MOTA	1647		LEU			84.716	45.787	2.326	1.00 17.24 A
	MOTA	1648		LEU			83.570	46.273	0.118	1.00 19.08 A
	MOTA	1649	C	LEU			83.050	42.025	-0.693	1.00 24.50 A
45	ATOM	1650	0	LEU			83.446	42.042	-1.852	1.00 24.85 A
	MOTA	1651	N	ILE			82.906	40.904	-0.002	1.00 24.71 A
	MOTA	1652	CA	ILE	Α	290	83.182	39.601	-0.570	1.00 25.86 A
	MOTA	1653	CB	ILE	Α	290	83.131	38.521	0.528	1.00 26.67 A
	MOTA	1654	CG2	ILE	Α	290	83.229	37.154	-0.087	1.00 27.57 A
50	ATOM	1655	CG1	ILE	Α	290	84.282	38.736	1.511	1.00 28.90 A
	ATOM	1656	CD1	ILE	Α	290	84.173	37.928	2.798	1.00 28.83 A
	ATOM	1657	C	ILE	А	290	82.127	39.303	-1.637	1.00 26.89 A
	ATOM	1658	ō	ILE			82.446	38.879	-2.757	1.00 26.18 A
	ATOM	1659	N	PHE			80.864	39.531	-1.294	1.00 27.48 A
55	ATOM	1660	CA	PHE			79.789	39.287	-2.249	1.00 28.46 A
	ATOM	1661	CB	PHE			78.434	39.587	-1.620	1.00 27.24 A
	ATOM	1662	CG	PHE			78.079	38.664	-0.496	1.00 27.24 A
				PHE				37.431		
	ATOM	1663					78.716		-0.365	1.00 26.90 A
	MOTA	1664	CD2	PHE	А	Z91	77.074	38.996	0.399	1.00 25.83 A

	MOTA	1665		PHE			78.353	36.545	0.637	1.00 27.02 A
	MOTA	1666	CE2	PHE			76.700	38.109	1.412	1.00 28.02 A
	MOTA	1667	CZ	PHE	Α	291	77.338	36.882	1.532	1.00 26.74 A
	MOTA	1668	C	PHE	Α	291	79.971	40.159	-3.467	1.00 29.11 A
5	ATOM	1669	0	PHE	Α	291	79.595	39.787	-4.584	1.00 30.18 A
	MOTA	1670	N	GLN	Α	292	80.559	41.324	-3.240	1.00 28.88 A
	ATOM	1671	CA	GLN	А	292	80.783	42.280	-4.304	1.00 30.00 A
	ATOM	1672	CB	GLN			81.215	43.604	-3.679	1.00 32.57 A
	ATOM	1673	CG	GLN			81.191	44.799	-4.599	1.00 35.12 A
10	ATOM	1674	CD	GLN			81.208	46.113	-3.817	1.00 38.65 A
	ATOM	1675		GLN			82.159	46.409	-3.078	1.00 39.67 A
	ATOM	1676		GLN			80.150	46.903	-3.972	1.00 38.94 A
	ATOM	1677	C	GLN			81.822	41.755	-5.296	1.00 28.96 A
	ATOM	1678	ō	GLN			81.633	41.844	-6.510	1.00 28.45 A
15	ATOM	1679	N	LYS			82.910	41.193	-4.787	1.00 26.32 A
13	ATOM	1680	CA	LYS			83.930	40.661	-5.669	1.00 26.32 A
	ATOM	1681	CB	LYS			85.174	40.319	-4.858	1.00 28.03 A
	MOTA	1682	CG	LYS			85.777	41.539	-4.177	1.00 28.52 A
	ATOM	1683	CD	LYS			87.065	41.208	-3.482	1.00 29.14 A
20	MOTA	1684	CE	LYS			87.912	42.449	-3.269	1.00 30.09 A
	MOTA	1685	NZ	LYS			89.165	42.157	-2.490	1.00 30.06 A
	MOTA	1686	C	LYS			83.414	39.432	-6.434	1.00 26.13 A
	MOTA	1687	0	LYS			83.721	39.231	-7.617	1.00 26.02 A
	MOTA	1688	N	ILE			82.617	38.621	-5.755	1.00 24.49 A
25	ATOM	1689	CA	ILE	А	294	82.047	37.429	-6.362	1.00 24.40 A
	ATOM	1690	CB	ILE	Α	294	81.168	36.680	-5.340	1.00 23.24 A
	MOTA	1691		ILE			80.154	35.763	-6.046	1.00 21.00 A
	MOTA	1692	CG1	ILE	Α	294	82.072	35.929	-4.365	1.00 19.23 A
	ATOM	1693	CD1	ILE	Α	294	81.388	35.559	-3.067	1.00 17.91 A
30	ATOM	1694	C	ILE	Α	294	81.224	37.744	-7.608	1.00 26.38 A
	ATOM	1695	0	ILE	Α	294	81.428	37.139	-8.661	1.00 25.96 A
	ATOM	1696	N	ILE			80.303	38.694	-7.505	1.00 28.38 A
	ATOM	1697	CA	ILE			79.467	39.018	-8.659	1.00 31.11 A
	ATOM	1698	CB	ILE			78.243	39.852	-8.248	1.00 31.46 A
35	ATOM	1699		ILE			77.548	39.181	-7.068	1.00 32.78 A
	ATOM	1700		ILE			78.669	41.268	-7.871	1.00 31.79 A
	ATOM	1701		ILE			77.518	42.132	-7.438	1.00 33.46 A
	ATOM	1702	C	ILE			80.201	39.731	-9.798	1.00 31.35 A
	ATOM	1703	Ö	ILE			79.709		-10.930	1.00 32.03 A
40	ATOM	1704	N	LYS			81.374	40.269	-9.511	1.00 30.68 A
40	ATOM	1705	CA	LYS			82.129		-10.552	1.00 30.66 A
	ATOM	1706	CB	LYS			82.683		-10.041	1.00 31.04 A
	ATOM	1707	CG	LYS			81.605	43.213	-9.520	1.00 32.01 A
45	ATOM	1708	CD	LYS			82.184	44.441	-8.841	1.00 37.38 A
43	MOTA	1709	CE	LYS			82.299	45.609	-9.803	1.00 40.30 A
	MOTA	1710	NZ	LYS			82.864	46.819	-9.119	1.00 42.94 A
	MOTA	1711	С	LYS			83.258		-10.966	1.00 31.87 A
	MOTA	1712	0	LYS			84.135		-11.745	1.00 32.98 A
	MOTA	1713	N	LEU			83.227		-10.443	1.00 30.62 A
50	MOTA	1714	CA	LEU			84.253		-10.735	1.00 29.78 A
	MOTA	1715	CB	LEU			84.100		-12.169	1.00 29.42 A
	MOTA	1716	CG	LEU			84.802		-12.527	1.00 29.13 A
	MOTA	1717		LEU			84.142	34.776	-11.783	1.00 27.91 A
	ATOM	1718	CD2	LEU	Α	297	84.725	35.682	-14.024	1.00 26.86 A
55	MOTA	1719	C	LEU	Α	297	85.622	38.436	-10.565	1.00 29.62 A
	ATOM	1720	0	LEU	Α	297	86.489	38.333	-11.419	1.00 28.99 A
	MOTA	1721	N	GLU	Α	298	85.807	39.091	-9.427	1.00 29.81 A
	MOTA	1722	CA	GLU			87.027	39.826	-9.143	1.00 30.88 A
	MOTA	1723	CB	GLU			86.622	41.166	-8.510	1.00 33.22 A

	ATOM	1724	CG	GLU	Α	298	87.754	42.136	-8.228	1.00	38.19 A	
	ATOM	1725	CD	GLU	Α	298	87.317	43.274	-7.303	1.00	41.34 A	
	ATOM	1726	OE1	GLU	Α	298	86.416	44.054	-7.684	1.00	43.93 A	
	ATOM	1727		GLU			87.867	43.382	-6.187		43.19 A	
5	ATOM	1728	C	GLU			88.071	39.110	-8.269		29.28 A	
	ATOM	1729	ŏ	GLU			88.066	39.230	-7.045		30.04 A	
	ATOM	1730	N	TYR			88.972	38.375	-8.906		26.46 A	
	ATOM	1731	CA	TYR			90.034	37.669	-8.194		26.46 A	
	MOTA	1732	CB	TYR			89.548	36.315	-7.640		24.23 A	
10	MOTA	1733	CG	TYR			89.403	35.252	-8.709		23.32 A	
	MOTA	1734	CD1	TYR	Α	299	88.369	35.318	-9.653	1.00	23.42 A	
	ATOM	1735	CE1	TYR	Α	299	88.274	34.392	-10.686	1.00	23.13 A	
	ATOM	1736	CD2	TYR	Α	299	90.337	34.227	-8.829	1.00	21.77 A	
	ATOM	1737	CE2	TYR	Α	299	90.250	33.292	-9.864	1.00	21.81 A	
15	ATOM	1738	CZ	TYR			89.214		-10.784		22.35 A	
	ATOM	1739	OH	TYR			89.089		-11.780		21.61 A	
	ATOM	1740	C	TYR			91.102	37.416	-9.245		28.31 A	
	ATOM	1741	ŏ	TYR			90.864		-10.426		27.25 A	
											30.57 A	
20	ATOM	1742	N	ASP		300	92.277	36.959	-8.844			
20	ATOM	1743	CA	ASP			93.282	36.687	-9.851		33.57 A	
	MOTA	1744	CB	ASP		300	94.012		-10.193		38.77 A	
	MOTA	1745	CG	ASP			94.382	38.768	-8.968		43.17 A	
	MOTA	1746		ASP			95.245	38.283	-8.197		46.59 A	
	ATOM	1747	OD2	ASP			93.802	39.865	-8.773		45.78 A	
25	MOTA	1748	C	ASP	Α	300	94.232	35.607	-9.364	1.00	33.20 A	
	ATOM	1749	0	ASP	Α	300	94.311	35.354	-8.169	1.00	33.46 A	
	MOTA	1750	N	PHE	Α	301	94.937	34.959	-10.287	1.00	32.16 A	
	ATOM	1751	CA	PHE	Α	301	95.853	33.892	-9.910	1.00	33.41 A	
	ATOM	1752	CB	PHE			95.922		-11.001		32.89 A	
30	ATOM	1753	CG	PHE		301	94.590		-11.403		33.05 A	
	ATOM	1754		PHE		301	93.763		-12.297		31.61 A	
	ATOM	1755	CD2	PHE			94.171		-10.905		30.94 A	
	ATOM	1756		PHE			92.548		-12.687		31.29 A	
		1757	CE2	PHE								
2.5	MOTA						92.961		-11.287		31.42 A	
35	ATOM	1758	CZ			301	92.142		-12.184		32.69 A	
	MOTA	1759	C	PHE			97.287	34.359	-9.649		34.23 A	
	MOTA	1760	0	PHE			97.784		-10.303		33.66 A	
	MOTA	1761	N	PRO			97.962	33.750	-8.665		35.45 A	
	MOTA	1762	CD	PRO	Α	302	97.426	32.932	-7.564	1.00	35.55 A	
40	MOTA	1763	CA	PRO	Α	302	99.347	34.145	-8.395	1.00	35.82 A	
	MOTA	1764	CB	PRO	Α	302	99.612	33.571	-7.009	1.00	35.09 A	
	ATOM	1765	CG	PRO	Α	302	98.682	32.401	-6.933	1.00	34.93 A	
	ATOM	1766	С	PRO	Α	302	100.214	33.506	-9.485	1.00	37.48 A	
	ATOM	1767	0	PRO	Α	302	99.830	32.504	-10.083	1.00	37.30 A	
45	ATOM	1768	N	ALA			101.370	34.100	-9.744		39.16 A	
	MOTA	1769	CA	ALA			102.293		-10.775		39.50 A	
	ATOM	1770	CB	ALA			103.612		-10.640		39.58 A	
	ATOM	1771	C	ALA			102.577		-10.832		41.05 A	
	ATOM	1772	Ö	ALA			102.642		-11.920		42.39 A	
50												
30	MOTA	1773	N	ALA			102.758	31.526	-9.671		40.38 A	
	MOTA	1774	CA	ALA			103.099	30.105	-9.614		39.93 A	
	MOTA	1775	CB	ALA			103.627	29.772	-8.212		41.64 A	
	MOTA	1776	C	ALA			102.025		-10.002		38.27 A	
	MOTA	1777	0	ALA			102.343		-10.453		39.29 A	
55	ATOM	1778	N	PHE			100.764	29.453	-9.813		35.83 A	
	MOTA	1779	CA	PHE	Α	305	99.614	28.587	-10.085	1.00	33.62 A	
	MOTA	1780	CB	PHE	Α	305	98.376	29.475	-10.278	1.00	32.70 A	
	MOTA	1781	CG			305	97.096	28.857	-9.796	1.00	31.41 A	
	ATOM	1782	CD1	PHE	Α	305	96.422	27.915	-10.574	1.00	30.30 A	

	ATOM	1783		PHE			96.556	29.225 -8.562	1.00 30.99 A
	ATOM	1784	CE1	PHE			95.230	27.350 -10.136	1.00 29.76 A
	MOTA	1785		PHE			95.352	28.663 -8.105	1.00 30.08 A
	MOTA	1786	CZ	PHE	Α	305	94.689	27.725 -8.897	1.00 30.22 A
5	ATOM	1787	C	PHE	Α	305	99.735	27.580 -11.241	1.00 32.03 A
	MOTA	1788	0	PHE	Α	305	99.767	27.962 -12.405	1.00 32.54 A
	ATOM	1789	N	PHE	Α	306	99.781	26.290 -10.914	1.00 31.58 A
	ATOM	1790	CA	PHE	А	306	99.886	25.235 -11.932	1.00 30.32 A
	ATOM	1791	CB	PHE		306	99.518	23.875 -11.338	1.00 29.86 A
10	ATOM	1792	CG	PHE		306	100.087	23.639 -9.971	1.00 30.29 A
	ATOM	1793		PHE		306	101.447	23.783 -9.733	1.00 30.37 A
	ATOM	1794	CD2	PHE		306	99.259	23.275 -8.919	1.00 30.23 A
	ATOM	1795		PHE		306	101.975	23.570 -8.465	1.00 30.23 A
	ATOM	1796	CE2	PHE		306	99.773	23.061 -7.648	1.00 30.90 A
15	ATOM	1797	CZ	PHE			101.136	23.210 -7.418	1.00 30.91 A
13	ATOM	1798	C	PHE			98.949	25.545 -13.096	1.00 31.14 A
	ATOM	1799	0	PHE			97.738	25.631 -12.920	1.00 30.39 A
	ATOM	1800	N	PRO		307	99.501	25.701 -14.309	1.00 28.76 A
20	ATOM	1801	CD	PRO			100.934	25.575 -14.635	1.00 27.67 A
20	ATOM	1802	CA	PRO			98.731	26.014 -15.520	1.00 27.24 A
	MOTA	1803	CB	PRO		307	99.757	25.848 -16.635	1.00 25.23 A
	MOTA	1804	CG	PRO		307	101.010	26.262 -15.978	1.00 25.61 A
	MOTA	1805	С	PRO			97.457	25.221 -15.787	1.00 25.86 A
	ATOM	1806	0	PRO			96.419	25.808 -16.098	1.00 24.65 A
25	ATOM	1807	N	LYS			97.521	23.901 -15.682	1.00 25.13 A
	ATOM	1808	CA	LYS		308	96.330	23.109 -15.952	1.00 24.53 A
	MOTA	1809	CB	LYS			96.689	21.640 -16.136	1.00 24.86 A
	MOTA	1810	CG	LYS	Α	308	97.361	21.413 -17.490	1.00 25.50 A
	ATOM	1811	CD	LYS	Α	308	97.987	20.047 -17.616	1.00 27.33 A
30	ATOM	1812	CE	LYS	Α	308	98.678	19.886 -18.961	1.00 29.39 A
	ATOM	1813	NZ	LYS	Α	308	99.232	18.505 -19.146	1.00 32.38 A
	ATOM	1814	С	LYS	Α	308	95.282	23.293 -14.890	1.00 24.82 A
	ATOM	1815	0	LYS	Α	308	94.085	23.281 -15.193	1.00 24.89 A
	ATOM	1816	N	ALA	Α	309	95.716	23.489 -13.647	1.00 24.73 A
35	ATOM	1817	CA	ALA	А	309	94.758	23.716 -12.573	1.00 25.03 A
	ATOM	1818	CB	ALA			95.445	23.662 -11.208	1.00 24.10 A
	ATOM	1819	C	ALA			94.140	25.094 -12.816	1.00 25.34 A
	ATOM	1820	ō	ALA			92.934	25.273 -12.679	1.00 26.34 A
	ATOM	1821	N	ARG			94.958	26.067 -13.198	1.00 26.07 A
40	ATOM	1822	CA	ARG			94.419	27.396 -13.453	1.00 28.32 A
	ATOM	1823	CB	ARG			95.513	28.359 -13.908	1.00 29.31 A
	ATOM	1824	CG	ARG			94.940	29.708 -14.288	1.00 31.58 A
	ATOM	1825	CD	ARG			95.917	30.588 -15.030	1.00 31.30 A
	ATOM	1826	NE	ARG			95.275	31.825 -15.473	1.00 34.52 A
45	ATOM	1827	CZ	ARG			95.771	33.050 -15.276	1.00 35.51 A
43	ATOM	1828		ARG			96.929	33.205 -14.633	
	ATOM	1829		ARG			95.106	34.124 -15.720	1.00 33.99 A 1.00 32.10 A
	ATOM	1830	C	ARG			93.331	27.348 -14.521	1.00 29.03 A
50	ATOM	1831	0	ARG			92.308	28.034 -14.418	1.00 29.32 A
50	MOTA	1832	N	ASP			93.548	26.536 -15.551	1.00 29.06 A
	MOTA	1833	CA	ASP			92.571	26.432 -16.620	1.00 29.87 A
	MOTA	1834	CB	ASP			93.156	25.636 -17.776	1.00 31.71 A
	MOTA	1835	CG	ASP			92.207	25.537 -18.953	1.00 34.71 A
	MOTA	1836		ASP		311	91.288	24.690 -18.912	1.00 36.90 A
55	MOTA	1837		ASP			92.378	26.312 -19.918	1.00 36.33 A
	MOTA	1838	C	ASP			91.264	25.800 -16.128	1.00 29.70 A
	MOTA	1839	0	ASP			90.169	26.238 -16.513	1.00 29.95 A
	MOTA	1840	N	LEU	Α	312	91.383	24.778 -15.282	1.00 26.64 A
	MOTA	1841	CA	LEU	Α	312	90.215	24.112 -14.715	1.00 24.92 A

	ATOM	1842	CB	LEU	Α	312	90.645	22.911 -13.869	1.00 23.9	3 A
	ATOM	1843	CG	LEU	Α	312	89.504	22.112 -13.227	1.00 24.4	8 A
	ATOM	1844	CD1	LEU	Α	312	88.569	21.610 -14.296	1.00 25.0	7 A
	ATOM	1845		LEU			90.061	20.945 -12.460	1.00 25.1	
5	ATOM	1846	C	LEU	A	312	89.412	25.095 -13.841	1.00 23.8	
	ATOM	1847	ō	LEU			88.182	25.136 -13.896	1.00 21.2	
	ATOM	1848	N	VAL			90.121	25.886 -13.042	1.00 23.1	
	ATOM	1849	CA	VAL			89.484	26.865 -12.171	1.00 23.5	
	MOTA	1850	CB	VAL			90.536	27.583 -11.297	1.00 22.3	
10	MOTA	1851		VAL			89.898	28.752 -10.559	1.00 19.0	
	MOTA	1852		VAL			91.144	26.607 -10.305	1.00 19.8	
	ATOM	1853	С	VAL	Α	313	88.701	27.915 -12.975	1.00 25.5	9 A
	ATOM	1854	0	VAL	Α	313	87.590	28.305 -12.605	1.00 26.5	7 A
	ATOM	1855	N	GLU	Α	314	89.278	28.378 -14.076	1.00 26.0	8 A
15	ATOM	1856	CA	GLU	Α	314	88.598	29.370 -14.895	1.00 26.7	9 A
	ATOM	1857	CB	GLU			89.543	29.928 -15.948	1.00 27.5	
	ATOM	1858	CG	GLU			90.739	30.639 -15.381	1.00 32.2	
	ATOM	1859	CD	GLU			91.687	31.094 -16.463	1.00 35.8	
	ATOM	1860		GLU			91.967		1.00 38.0	
20								30.280 -17.375		
20	ATOM	1861	OE2	GLU			92.157	32.257 -16.399	1.00 38.4	
	MOTA	1862	C	GLU			87.370	28.787 -15.577	1.00 26.2	
	MOTA	1863	0	GLU			86.499	29.527 -16.038	1.00 27.2	
	ATOM	1864	N	LYS			87.300	27.464 -15.662	1.00 24.7	
	MOTA	1865	CA	LYS			86.151	26.832 -16.294	1.00 23.€	
25	ATOM	1866	CB	LYS	Α	315	86.578	25.584 -17.073	1.00 23.6	9 A
	ATOM	1867	CG	LYS	Α	315	87.393	25.865 -18.344	1.00 22.4	1 A
	ATOM	1868	CD	LYS	Α	315	87.825	24.545 -18.968	1.00 25.6	8 A
	ATOM	1869	CE	LYS	Α	315	88.768	24.695 -20.155	1.00 24.8	6 A
	ATOM	1870	NZ	LYS	А	315	88.082	25.219 -21.346	1.00 28.6	2 A
30	ATOM	1871	C	LYS			85.119	26.471 -15.230	1.00 23.4	
	ATOM	1872	ō	LYS			84.043	25.970 -15.541	1.00 25.3	
	ATOM	1873	N	LEU			85.454	26.730 -13.970	1.00 21.8	
	ATOM	1874	CA	LEU			84.549	26.461 -12.862	1.00 20.2	
	ATOM	1875	CB	LEU			85.272	25.705 -11.767	1.00 20.2	
25										
35	ATOM	1876	CG	LEU			85.409	24.221 -12.078	1.00 21.1	
	MOTA	1877		LEU			86.272	23.552 -11.009	1.00 19.2	
	MOTA	1878		LEU			84.000	23.600 -12.166	1.00 18.5	
	MOTA	1879	С	LEU			83.996	27.758 -12.290	1.00 21.3	
	MOTA	1880	0	LEU	А	316	82.811	27.848 -11.955	1.00 18.7	9 A
40	MOTA	1881	N	LEU	Α	317	84.865	28.762 -12.175	1.00 20.5	9 A
	ATOM	1882	CA	LEU	Α	317	84.446	30.038 -11.646	1.00 21.6	4 A
	ATOM	1883	CB	LEU	Α	317	85.606	30.707 -10.900	1.00 21.4	2 A
	ATOM	1884	CG	LEU	А	317	86.130	29.892 -9.711	1.00 21.8	0 A
	ATOM	1885	CD1	LEU			87.299	30.599 -9.047	1.00 23.0	
45	ATOM	1886		LEU			85.031	29.688 -8.724	1.00 20.3	
	ATOM	1887	C	LEU			83.940	30.890 -12.810	1.00 23.3	
	ATOM	1888	Ö	LEU			84.568	31.859 -13.242	1.00 23.2	
	ATOM	1889	N	VAL			82.786	30.485 -13.324	1.00 24.0	
50	ATOM	1890	CA	VAL			82.135	31.161 -14.436	1.00 23.4	
50	MOTA	1891	CB	VAL			81.829	30.150 -15.547	1.00 24.3	
	MOTA	1892		VAL			81.061	30.828 -16.670	1.00 22.5	
	MOTA	1893		VAL			83.136	29.524 -16.049	1.00 20.6	
	MOTA	1894	C	VAL			80.838	31.765 -13.918	1.00 24.5	
	MOTA	1895	0	VAL			80.050	31.086 -13.250	1.00 24.8	
55	ATOM	1896	N	LEU	Α	319	80.603	33.036 -14.215	1.00 24.9	5 A
	ATOM	1897	CA	LEU	Α	319	79.383	33.688 -13.731	1.00 25.7	9 A
	ATOM	1898	CB	LEU		319	79.379	35.157 -14.154	1.00 25.3	
	ATOM	1899	CG	LEU			80.466	35.963 -13.417	1.00 27.0	
	ATOM	1900		LEU			80.452	37.421 -13.869	1.00 25.5	

	ATOM	1901		LEU A		80.241		-11.907		23.27 A
	ATOM	1902	C	LEU A		78.077		-14.141		26.05 A
	MOTA	1903	0	LEU A		77.171		-13.319		27.69 A
-	ATOM	1904	N	ASP A		77.982		-15.400		25.08 A
5	MOTA	1905	CA	ASP A		76.804		-15.892		24.00 A
	MOTA	1906	CB	ASP A		76.788		-17.420		24.02 A
	MOTA	1907	CG	ASP A		75.597		-17.996		27.27 A
	MOTA	1908		ASP A		75.009		-17.271		29.66 A
	MOTA	1909		ASP A		75.253		-19.175		30.03 A
10	MOTA	1910	C	ASP A		76.846		-15.396		24.04 A
	ATOM	1911	0	ASP A		77.661		-15.846		25.11 A
	ATOM	1912	N	ALA A		75.940		-14.489		23.73 A
	MOTA	1913	CA	ALA A		75.867		-13.887		23.58 A
	ATOM	1914	CB	ALA A		74.710		-12.916		23.62 A
15	MOTA	1915	C	ALA A	321	75.765	27.599	-14.853	1.00	24.90 A
	ATOM	1916	0	ALA A	321	76.221	26.497	-14.549	1.00	24.36 A
	ATOM	1917	N	THR A	322	75.176	27.834	-16.019	1.00	25.50 A
	MOTA	1918	CA	THR A	322	75.008	26.772	-17.011	1.00	24.60 A
	MOTA	1919	CB	THR A	322	73.816	27.064	-17.909	1.00	23.09 A
20	MOTA	1920	OG1	THR A	322	74.079	28.263	-18.646	1.00	23.74 A
	ATOM	1921	CG2	THR A	322	72.568	27.260	-17.080	1.00	20.71 A
	ATOM	1922	С	THR A	322	76.238	26.596	-17.893	1.00	25.24 A
	ATOM	1923	0	THR A	322	76.221	25.807	-18.832	1.00	26.45 A
	ATOM	1924	N	LYS A		77.300		-17.592		25.05 A
25	MOTA	1925	CA	LYS A		78.526		-18.366		26.46 A
	MOTA	1926	CB	LYS A		78.972		-18.823		28.68 A
	ATOM	1927	CG	LYS A		78.050		-19.814		31.27 A
	ATOM	1928	CD	LYS A		78.470		-21.240		34.38 A
	ATOM	1929	CE	LYS A		77.850		-22.243		35.12 A
30	ATOM	1930	NZ	LYS A		76.363		-22.251		36.71 A
	ATOM	1931	C	LYS A		79.660		-17.556		26.39 A
	ATOM	1932	0	LYS A		80.795		-18.010		28.51 A
	ATOM	1933	N	ARG A		79.372		-16.360		24.50 A
	ATOM	1934	CA	ARG A		80.429		-15.543		23.37 A
35	ATOM	1935	CB	ARG A		80.087		-14.049		23.41 A
	ATOM	1936	CG	ARG A		80.233		-13.520		21.60 A
	ATOM	1937	CD	ARG A		79.594		-12.173		21.55 A
	ATOM	1938	NE	ARG A		79.245		-11.986		19.69 A
	ATOM	1939	CZ	ARG A		78.273		-11.191		19.84 A
40	ATOM	1940		ARG A		77.555		-10.496		16.83 A
	ATOM	1941		ARG A		77.990		-11.129		21.41 A
	ATOM	1942	С	ARG A		80.717		-15.897		22.63 A
	ATOM	1943	o	ARG A		79.798		-16.058		24.44 A
	ATOM	1944	N	LEU A		82.000		-16.023		20.68 A
45	ATOM	1945	CA	LEU A		82.414		-16.352		20.98 A
	ATOM	1946	CB	LEU A		83.952		-16.386		20.82 A
	ATOM	1947	CG	LEU A		84.596		-17.131		23.08 A
	ATOM	1948		LEU A		84.149		-18.595		21.39 A
	ATOM	1949		LEU A		86.132		-17.038		20.00 A
50	ATOM	1950	C	LEU A		81.840		-15.290		20.43 A
50	ATOM	1951	0	LEU A		82.062		-14.097		18.45 A
	MOTA	1952 1953	N	GLY A		81.076 80.501		-15.725 -14.778		21.33 A 20.60 A
	ATOM		CA							
	ATOM	1954	C	GLY A		78.984		-14.701		22.39 A
55	ATOM	1955	0	GLY A		78.383		-14.378		22.59 A
	ATOM	1956	N	CYS A		78.358		-15.009		23.36 A
	ATOM	1957	CA	CYS A		76.896		-14.963		25.18 A
	ATOM	1958	CB	CYS A		76.453		-14.889		25.79 A
	MOTA	1959	SG	CYS A	321	76.742	23.237	-16.364	1.00	31.42 A

	MOTA	1960	C	CYS	Α	327	76.229	20.074 -16.148	1.00 24.99 A
	MOTA	1961	0	CYS	Α	327	76.887	19.743 -17.129	1.00 24.31 A
	MOTA	1962	N	ALA	Α	328	74.923	19.847 -16.040	1.00 26.34 A
	ATOM	1963	CA	ALA	Α	328	74.157	19.172 -17.094	1.00 27.51 A
5	ATOM	1964	CB	ALA	Α	328	72.703	18.949 -16.629	1.00 26.81 A
	ATOM	1965	C	ALA	А	328	74.179	19.905 -18.443	1.00 28.11 A
	ATOM	1966	o	ALA			74.243	19.274 -19.501	1.00 27.66 A
	ATOM	1967	N	GLU			74.144	21.231 -18.418	1.00 28.05 A
	ATOM	1968	CA	GLU			74.172	21.973 -19.668	1.00 29.54 A
10	ATOM	1969	CB	GLU			73.915	23.458 -19.428	1.00 32.18 A
10	ATOM	1970	CG	GLU			72.539	23.783 -18.863	1.00 37.89 A
	ATOM	1971	CD	GLU			72.418	23.503 -17.374	1.00 41.37 A
	MOTA	1972		GLU			73.464	23.308 -16.711	1.00 43.80 A
	MOTA	1973					71.273	23.495 -16.863	1.00 43.66 A
15	MOTA	1974	C	GLU		329	75.514	21.807 -20.377	1.00 29.08 A
	MOTA	1975	0	GLU			75.602	21.927 -21.605	1.00 27.73 A
	MOTA	1976	N	MET			76.559	21.540 -19.598	1.00 27.54 A
	MOTA	1977	CA	MET	Α	330	77.894	21.359 -20.148	1.00 25.71 A
	MOTA	1978	CB	MET	Α	330	78.945	21.963 -19.219	1.00 27.88 A
20	ATOM	1979	CG	MET	Α	330	78.964	23.489 -19.209	1.00 30.29 A
	ATOM	1980	SD	MET	Α	330	79.429	24.194 -20.819	1.00 34.04 A
	MOTA	1981	CE	MET	Α	330	81.187	23.670 -20.936	1.00 29.55 A
	ATOM	1982	C	MET	Α	330	78.156	19.884 -20.343	1.00 24.53 A
	ATOM	1983	o	MET			79.290	19.473 -20.575	1.00 22.65 A
25	ATOM	1984	N	GLU			77.089	19.095 -20.221	1.00 22.87 A
	ATOM	1985	CA	GLU			77.139	17.654 -20.415	1.00 21.38 A
	ATOM	1986	CB	GLU			77.854	17.339 -21.735	1.00 22.71 A
	ATOM	1987	CG	GLU			76.903	16.916 -22.837	1.00 23.01 A
	ATOM	1988	CD	GLU			75.599	17.720 -22.875	1.00 24.76 A
30	ATOM	1989		GLU			75.570	18.830 -23.441	1.00 24.76 A
30	ATOM	1990		GLU			74.588	17.230 -22.337	1.00 24.22 A
			C	GLU			77.671	16.765 -19.290	1.00 24.22 A
	ATOM	1991							
	MOTA	1992	0	GLU			78.075	15.619 -19.517	1.00 19.50 A
	MOTA	1993	N	GLY			77.675	17.284 -18.071	1.00 19.73 A
35	MOTA	1994	CA	GLY			78.056	16.445 -16.954	1.00 17.80 A
	MOTA	1995	C	GLY			79.494	16.243 -16.570	1.00 17.28 A
	MOTA	1996	0	GLY			80.381	17.013 -16.934	1.00 16.11 A
	MOTA	1997	N	TYR			79.701	15.151 -15.842	1.00 16.52 A
	MOTA	1998	CA	TYR	Α	333	80.997	14.791 -15.305	1.00 16.75 A
40	MOTA	1999	CB	TYR	Α	333	80.787	13.854 -14.115	1.00 16.95 A
	MOTA	2000	CG	TYR	Α	333	80.369	14.624 -12.893	1.00 18.08 A
	MOTA	2001	CD1	TYR	Α	333	81.332	15.207 -12.059	1.00 18.77 A
	ATOM	2002	CE1	TYR	Α	333	80.971	16.035 -10.982	1.00 17.69 A
	ATOM	2003	CD2	TYR	Α	333	79.021	14.877 -12.620	1.00 17.08 A
45	ATOM	2004	CE2	TYR	Α	333	78.646	15.713 -11.538	1.00 19.05 A
	ATOM	2005	CZ	TYR	Α	333	79.640	16.287 -10.728	1.00 18.04 A
	ATOM	2006	OH	TYR	А	333	79.322	17.126 -9.682	1.00 18.69 A
	ATOM	2007	C	TYR			82.051	14.240 -16.238	1.00 16.78 A
	ATOM	2008	ō	TYR			83.248	14.393 -15.977	1.00 16.04 A
50	ATOM	2009	N	GLY			81.633	13.598 -17.321	1.00 16.63 A
50	ATOM	2010	CA	GLY			82.624	13.082 -18.244	1.00 17.02 A
	ATOM	2011	C	GLY			83.576	14.194 -18.683	1.00 17.02 A
	ATOM	2011	0	GLY			84.802	14.194 -18.562	1.00 17.47 A
55	ATOM	2013	N	PRO			83.039	15.315 -19.195	1.00 17.04 A
33	ATOM	2014	CD	PRO			81.650	15.611 -19.590	1.00 16.18 A
	MOTA	2015	CA	PRO			83.940	16.382 -19.621	1.00 17.35 A
	MOTA	2016	CB	PRO		335	82.991	17.441 -20.178	1.00 17.48 A
	MOTA	2017	CG			335	81.857	16.605 -20.713	1.00 18.64 A
	ATOM	2018	C	PRO	Α	335	84.786	16.883 -18.480	1.00 18.48 A

	ATOM	2019	0	PRO	Α	335	85.963	17.131	-18.661	1.00	20.84	A
	MOTA	2020	N	LEU	А	336	84.204	17.034	-17.299	1.00	19.46 2	A
	MOTA	2021	CA	LEU	А	336	84.986		-16.153		19.38 2	
	ATOM	2022	CB	LEU			84.071		-14.937		18.98	
5	ATOM	2023	CG	LEU			84.765		-13.604		18.01	
-	ATOM	2024		LEU			85.534		-13.690		16.66	
	ATOM	2025		LEU			83.724		-12.491		18.81	
	ATOM	2026	C	LEU			86.132		-15.815		19.32	
		2027		LEU			87.293		-15.683		18.65	
1.0	ATOM		0									
10	MOTA	2028	N	LYS			85.808		-15.688		18.38 2	
	MOTA	2029	CA	LYS			86.821		-15.387		18.89	
	MOTA	2030	CB	LYS			86.147		-15.082		17.70 2	
	MOTA	2031	CG	LYS			85.460		-13.727		19.89 2	
	MOTA	2032	CD	LYS			84.450		-13.523		22.66 2	
15	MOTA	2033	CE	LYS	Α	337	85.089	10.453	-13.372	1.00	22.78 2	A
	MOTA	2034	NZ	LYS	Α	337	84.025	9.444	-13.088	1.00	25.28 2	A
	MOTA	2035	C	LYS	Α	337	87.865	14.101	-16.504	1.00	20.07 2	Α
	MOTA	2036	0	LYS	Α	337	88.996	13.671	-16.254	1.00	20.47 2	A
	MOTA	2037	N	ALA	Α	338	87.491	14.486	-17.725	1.00	20.38 2	A
20	MOTA	2038	CA	ALA			88.393		-18.876	1.00	20.65 2	A
	MOTA	2039	CB	ALA			87.580	14.382	-20.178		20.29 2	
	ATOM	2040	С	ALA			89.357		-18.933		22.18	
	ATOM	2041	ō	ALA			90.265		-19.768		24.71 2	
	ATOM	2042	N	HIS			89.179		-18.063		21.90 2	
25	ATOM	2043	CA	HIS			90.072		-18.094		22.10 2	
	ATOM	2044	CB	HIS			89.711		-16.989		21.35 2	
	ATOM	2045	CG	HIS			90.357		-17.149		20.57	
	ATOM	2045		HIS			89.891		-17.143		19.19	
		2047		HIS			91.664		-16.783		20.52	
30	ATOM	2047		HIS			91.664		-16.783		22.28	
30	ATOM											
	ATOM	2049		HIS			90.914		-17.633		21.96 2	
	MOTA	2050	С	HIS			91.555		-17.963		22.78	
	MOTA	2051	0	HIS			91.919		-17.118		21.05 2	
	MOTA	2052	N	PRO			92.425		-18.801		24.12 2	
35	MOTA	2053	CD	PRO			92.090		-19.855		23.53 2	
	MOTA	2054	CA	PRO			93.872		-18.795		25.11 2	
	MOTA	2055	CB	PRO			94.435		-19.647		22.31 2	
	MOTA	2056	CG	PRO			93.379		-20.685		22.50 2	
	MOTA	2057	С	PRO	Α	340	94.540	17.654	-17.421	1.00	25.66 2	A
40	MOTA	2058	0	PRO	Α	340	95.523	16.951	-17.237	1.00	27.43 2	A
	MOTA	2059	N	PHE	Α	341	94.011	18.389	-16.459	1.00	25.05 2	A
	MOTA	2060	CA	PHE	Α	341	94.596	18.399	-15.139	1.00	24.88 2	A
	MOTA	2061	CB	PHE	Α	341	93.897	19.459	-14.276	1.00	24.71 2	A
	MOTA	2062	CG	PHE	Α	341	94.482	19.607	-12.893	1.00	24.42 2	A
45	ATOM	2063	CD1	PHE	Α	341	95.822	19.947	-12.721	1.00	22.55 2	A
	MOTA	2064	CD2	PHE	А	341	93.685	19.397	-11.758	1.00	22.61 2	A
	MOTA	2065		PHE			96.364		-11.434		23.65 2	
	MOTA	2066		PHE			94.204		-10.476		22.09 2	
	ATOM	2067	CZ	PHE			95.547		-10.304		24.01 2	
50	ATOM	2068	c	PHE			94.511		-14.486		25.70 2	
	ATOM	2069	ō	PHE			95.363		-13.680		27.11	
	ATOM	2070	N	PHE			93.499		-14.865		25.51	
	ATOM	2071	CA	PHE			93.262		-14.318		25.34	
	ATOM	2071	CB	PHE			91.758		-14.318		21.93	
55		2072		PHE					-14.120		20.26	
33	MOTA		CG CD1				91.120					
	ATOM	2074		PHE			91.556		-11.888		20.03 2	
	MOTA	2075		PHE			90.030		-13.613		19.36	
	MOTA	2076		PHE			90.907		-11.004		19.87	
	MOTA	2077	CE2	PHE	Α	342	89.377	17.348	-12.744	1.00	18.17	A

	ATOM	2078	CZ	PHE			89.818	17.470 -1			19.27	
	ATOM	2079	C	PHE			93.805	13.815 -1			27.64	
	MOTA	2080	0	PHE			93.508	12.630 -1		1.00	27.39	Α
	MOTA	2081	N	GLU	Α	343	94.607	14.203 -1	6.194	1.00	31.32	Α
5	ATOM	2082	CA	GLU	А	343	95.185	13.262 -1	7.150	1.00	34.29	Α
	ATOM	2083	CB	GLU	А	343	96.320	13.950 -1	7.889	1.00	38.36	А
	ATOM	2084	CG	GLU			96.735	13.314 -1			45.23	
	ATOM	2085	CD	GLU			97.654	14.247 -1			51.01	
	ATOM	2086		GLU			98.266	13.801 -2			51.76	
10												
10	ATOM	2087		GLU			97.755	15.439 -1			52.42	
	MOTA	2088	C	GLU			95.690	11.950 -1			33.50	
	ATOM	2089	0	GLU			95.289	10.860 -1			33.57	
	MOTA	2090	N	SER			96.554	12.049 -1			31.58	
	ATOM	2091	CA	SER	Α	344	97.117	10.857 -1	4.906	1.00	30.38	Α
15	MOTA	2092	CB	SER	Α	344	98.447	11.217 -1	4.253	1.00	29.76	Α
	ATOM	2093	OG	SER	Α	344	98.243	11.995 -1	3.096	1.00	30.32	А
	ATOM	2094	C	SER			96.242	10.150 -1			30.00	
	ATOM	2095	ō	SER			96.662	9.137 -1			31.14	
	ATOM	2096	N	VAL			95.046	10.679 -1			27.28	
20	ATOM	2097	CA	VAL			94.135	10.126 -1			25.39	
20											24.17	
	ATOM	2098	CB	VAL			93.093	11.213 -1				
	MOTA	2099		VAL			91.973	10.568 -1			19.50	
	MOTA	2100		VAL			93.779	12.321 -1			17.85	
	MOTA	2101	С	VAL			93.341	8.885 -1			26.45	
25	ATOM	2102	0	VAL	А	345	92.813	8.842 -1			27.42	
	MOTA	2103	N	THR	Α	346	93.253	7.890 -1	2.157	1.00	26.62	Α
	ATOM	2104	CA	THR	Α	346	92.451	6.680 -1	2.406	1.00	27.91	Α
	ATOM	2105	CB	THR	А	346	93.194	5.388 -1	1.999		29.18	
	ATOM	2106	OG1	THR	А	346	94.345	5.224 -1	2.830	1.00	33.51	А
30	ATOM	2107		THR			92.300	4.171 -1			28.24	
	ATOM	2108	C	THR			91.229	6.856 -1			27.53	
	ATOM	2109	Ö	THR			91.297	6.621 -1			29.24	
	ATOM	2110	N	TRP			90.117	7.279 -1			27.83	
2.5	ATOM	2111	CA	TRP			88.898	7.561 -1			29.15	
35	MOTA	2112	CB	TRP			87.878	8.278 -1			27.12	
	ATOM	2113	CG	TRP			88.353	9.574 -1			25.48	
	MOTA	2114		TRP			88.252	10.853 -1			24.27	
	MOTA	2115		TRP			88.841	11.803 -1			23.82	
	MOTA	2116	CE3	TRP	А	347	87.723	11.292 -1	0.897	1.00	22.42	Α
40	ATOM	2117	CD1	TRP	Α	347	88.984	9.788 -1	3.952	1.00	24.47	A
	ATOM	2118	NE1	TRP	Α	347	89.279	11.124 -1	4.099	1.00	23.92	Α
	ATOM	2119	CZ2	TRP	А	347	88.913	13.169 -1	2.678	1.00	21.68	Α
	ATOM	2120		TRP			87.797	12.654 -1			24.15	
	ATOM	2121		TRP			88.391	13.575 -1			22.35	
45	ATOM	2122	С	TRP			88.218	6.370 -1			30.64	
	ATOM	2123	ō	TRP			87.617		9.631		31.21	
	ATOM	2124		GLU			88.318	5.242 -1			32.16	
			N									
	MOTA	2125	CA	GLU			87.698	4.003 -1			34.98	
	MOTA	2126	CB	GLU			88.157	2.890 -1			37.47	
50	MOTA	2127	CG	GLU			87.815	3.125 -1			41.39	
	MOTA	2128	CD	GLU			88.619	4.257 -1			41.83	
	MOTA	2129		GLU			89.828	4.408 -1			42.27	
	ATOM	2130	OE2	GLU	Α	348	88.036	4.982 -1	4.959	1.00	42.41	A
	MOTA	2131	C	GLU	Α	348	87.843	3.547 -	9.478	1.00	34.74	Α
55	ATOM	2132	0	GLU	Α	348	86.866	3.111 -	8.869	1.00	35.95	A
	ATOM	2133	N	ASN	Α	349	89.024	3.652 -	8.887	1.00	33.61	Α
	ATOM	2134	CA	ASN			89.189		7.507		32.34	
	ATOM	2135	CB	ASN			89.936		7.529		33.21	
	ATOM	2136	CG	ASN			91.345		8.089		34.48	
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	ATOM	2137		ASN			91.613	2.943	-8.858	1.00 32.91 A
	MOTA	2138	ND2	ASN	Α	349	92.247	1.110	-7.712	1.00 35.85 A
	MOTA	2139	C	ASN	Α	349	89.949	4.136	-6.594	1.00 31.22 A
	MOTA	2140	0	ASN	Α	349	90.826	3.714	-5.839	1.00 31.07 A
5	ATOM	2141	N	LEU	Α	350	89.611	5.416	-6.646	1.00 28.54 A
	MOTA	2142	CA	LEU	Α	350	90.300	6.403	-5.837	1.00 26.75 A
	ATOM	2143	СВ	LEU			89.632	7.762	-6.024	1.00 25.89 A
	ATOM	2144	CG	LEU			90.095	8.558	-7.239	1.00 24.21 A
	ATOM	2145		LEU			89.111	9.674	-7.547	1.00 23.55 A
10	ATOM	2146		LEU			91.475	9.118	-6.932	1.00 23.67 A
	ATOM	2147	C	LEU			90.440	6.102	-4.345	1.00 27.67 A
	ATOM	2148	o	LEU			91.478	6.401	-3.753	1.00 28.06 A
	ATOM	2149	N	HIS			89.424	5.509	-3.722	1.00 27.81 A
	ATOM	2150	CA	HIS			89.539	5.254	-2.299	1.00 27.81 A
1.5										
15	MOTA	2151	CB	HIS			88.144	5.197	-1.646	1.00 31.47 A
	ATOM	2152	CG	HIS			87.584	3.823	-1.475	1.00 32.65 A
	MOTA	2153		HIS			86.926	3.009	-2.338	1.00 34.75 A
	MOTA	2154		HIS			87.629	3.150	-0.273	1.00 34.31 A
	MOTA	2155		HIS			87.022	1.981	-0.402	1.00 36.41 A
20	MOTA	2156		HIS			86.586	1.871	-1.644	1.00 35.36 A
	MOTA	2157	C	HIS			90.396	4.030	-1.978	1.00 30.93 A
	MOTA	2158	0	HIS	Α	351	90.674	3.741	-0.812	1.00 31.57 A
	MOTA	2159	N	GLN	Α	352	90.842	3.337	-3.022	1.00 31.09 A
	MOTA	2160	CA	GLN	Α	352	91.709	2.177	-2.864	1.00 31.86 A
25	ATOM	2161	CB	GLN	Α	352	91.482	1.187	-3.992	1.00 35.63 A
	MOTA	2162	CG	GLN	Α	352	91.038	-0.141	-3.497	1.00 40.62 A
	ATOM	2163	CD	GLN	Α	352	89.739	-0.036	-2.766	1.00 42.39 A
	ATOM	2164	OE1	GLN	А	352	88.684	0.133	-3.376	1.00 44.19 A
	ATOM	2165	NE2	GLN	А	352	89.802	-0.112	-1.447	1.00 44.81 A
30	ATOM	2166	С	GLN			93.167	2.626	-2.907	1.00 31.39 A
	ATOM	2167	o	GLN			94.030	2.022	-2.271	1.00 31.44 A
	ATOM	2168	N	GLN			93.429	3.685	-3.672	1.00 29.13 A
	ATOM	2169	CA	GLN			94.769	4.237	-3.813	1.00 27.37 A
	ATOM	2170	CB	GLN			94.767	5.283	-4.932	1.00 25.81 A
35	ATOM	2171	CG			353	94.250	4.702	-6.242	1.00 26.68 A
33	ATOM	2172	CD	GLN			94.035	5.738	-7.330	1.00 26.81 A
	ATOM	2173		GLN			94.792	6.709	-7.435	1.00 25.21 A
	ATOM	2174		GLN			93.011	5.520	-8.171	1.00 24.24 A
		2175	C			353	95.288	4.851	-2.510	1.00 24.24 A
40	ATOM	2176								
40	MOTA		0	GLN			94.511	5.245	-1.633	1.00 28.38 A
	MOTA	2177	N	THR			96.608	4.907	-2.375	1.00 28.16 A
	MOTA	2178	CA	THR			97.220	5.489	-1.193	1.00 28.54 A
	MOTA	2179	CB	THR			98.564	4.848	-0.889	1.00 29.50 A
	MOTA	2180		THR			98.354	3.459	-0.624	1.00 31.62 A
45	MOTA	2181		THR			99.225	5.517	0.334	1.00 27.68 A
	MOTA	2182	C	THR			97.438	6.955	-1.468	1.00 27.76 A
	MOTA	2183	0	THR			98.062	7.307	-2.453	1.00 27.12 A
	MOTA	2184	N	PRO			96.928	7.832	-0.592	1.00 28.37 A
	MOTA	2185	CD	PRO	Α	355	96.067	7.582	0.573	1.00 27.67 A
50	MOTA	2186	CA	PRO			97.092	9.266	-0.802	1.00 28.53 A
	MOTA	2187	CB	PRO	Α	355	96.215	9.883	0.291	1.00 28.29 A
	ATOM	2188	CG	PRO	Α	355	95.210	8.807	0.579	1.00 28.38 A
	ATOM	2189	C	PRO	Α	355	98.528	9.724	-0.695	1.00 28.85 A
	MOTA	2190	0	PRO	Α	355	99.290	9.232	0.139	1.00 29.42 A
55	ATOM	2191	N	PRO	Α	356	98.916	10.676	-1.548	1.00 28.20 A
	ATOM	2192	CD			356	98.083	11.340	-2.567	1.00 27.35 A
	ATOM	2193	CA			356	100.276	11.213	-1.539	1.00 28.63 A
	ATOM	2194	CB			356	100.261	12.199	-2.712	1.00 29.02 A
	ATOM	2195	CG			356	98.815	12.633	-2.781	1.00 27.44 A

	ATOM	2196	C	PRO	Α	356	100.483	11.899	-0.195	1.00 29.18 A
	ATOM	2197	0	PRO	Α	356	99.543	12.505	0.331	1.00 28.80 A
	ATOM	2198	N	ALA	Α	357	101.689	11.806	0.368	1.00 29.69 A
	ATOM	2199	CA	ALA			101.942	12.439	1.664	1.00 31.97 A
5	ATOM	2200	CB	ALA	А	357	103.273	11.964	2.253	1.00 29.11 A
	MOTA	2201	C	ALA			101.928	13.964	1.528	1.00 33.61 A
	ATOM	2201	0	ALA			102.371	14.507	0.520	1.00 33.81 A
	MOTA	2203	N			358	101.390	14.645	2.540	1.00 36.37 A
	MOTA	2204	CA	LEU			101.295	16.110	2.543	1.00 38.03 A
10	MOTA	2205	CB			358	99.995	16.554	3.209	1.00 36.49 A
	MOTA	2206	CG	LEU	Α	358	98.679	16.059	2.641	1.00 35.57 A
	ATOM	2207	CD1	LEU	Α	358	97.568	16.398	3.620	1.00 35.78 A
	ATOM	2208	CD2	LEU	Α	358	98.443	16.689	1.278	1.00 37.10 A
	ATOM	2209	С	LEU	А	358	102.460	16.743	3.310	1.00 39.05 A
15	ATOM	2210	0	LEU		358	102.451	16.592	4.553	1.00 39.24 A
	ATOM	2211		LEU		358	103.348	17.370	2.679	1.00 40.12 A
	ATOM	2212	OH2	TIP	s	1	82.347	32.462	-3.850	1.00 16.08 S
	ATOM	2213	OH2	TIP	S	4	80.761		-18.244	1.00 23.37 S
						7				
20	ATOM	2214	OH2	TIP	S		79.269		-18.353	1.00 22.32 S
20	MOTA	2215	OH2	TIP	S	8	86.710	32.919	-1.646	1.00 24.05 S
	MOTA	2216	OH2	TIP	S	9	78.564	-0.823	16.465	1.00 28.00 S
	MOTA	2217	OH2	TIP	S	10	75.323	16.274	8.538	1.00 18.43 S
	ATOM	2218		TIP	S	12	78.540	24.328	-2.128	1.00 27.08 S
	MOTA	2219	OH2	TIP	s	13	91.533	13.928	-17.231	1.00 22.56 S
25	ATOM	2220	OH2	TIP	s	14	77.419	-0.445	24.044	1.00 23.98 S
	ATOM	2221	OH2	TIP	s	19	72.498	40.164	-3.114	1.00 21.78 S
	ATOM	2222	OH2	TIP	S	20	77.303	13.198	-15.393	1.00 22.49 S
	MOTA	2223	OH2	TIP	s	21	75.600	-1.063	22.040	1.00 24.29 S
	ATOM	2224			s	22	90.133	19.697	12.606	1.00 16.61 S
30	ATOM	2225	OH2	TIP	s	24	74.810	7.002	5.700	1.00 20.66 S
30	ATOM	2226		TIP	s	27	74.894	8.778	-8.074	1.00 23.31 S
	ATOM	2227	OH2	TIP	S	28	80.070		-17.170	1.00 23.31 S
	MOTA	2228		TIP	S	31	74.744	21.007	3.348	1.00 29.98 S
	MOTA	2229	OH2	TIP	S	32	97.930	12.301	2.472	1.00 16.75 S
35	MOTA	2230	OH2	TIP	s	35	78.412	7.338	3.002	1.00 16.51 S
	ATOM	2231	OH2	TIP	s	36	80.172	27.171	1.300	1.00 34.66 S
	MOTA	2232	OH2	TIP	S	41	69.773	3.412	17.444	1.00 24.08 S
	ATOM	2233	OH2	TIP	S	43	88.878	7.904	10.616	1.00 20.34 S
	ATOM	2234	OH2	TIP	S	44	87.375	32.487	-13.928	1.00 31.99 S
40	ATOM	2235	OH2	TIP	s	45	91.671	10.803	-16.123	1.00 35.59 S
	ATOM	2236	OH2	TIP	s	46	87.637	11.564	23.703	1.00 22.67 S
	ATOM	2237	OH2	TIP	S	48	93.353	28.739	3.547	1.00 32.79 S
	ATOM	2238		TIP	S	50	82.283		-16.032	1.00 23.90 S
	ATOM	2239	OH2	TIP	s	52	81.673	8.965	-8.348	1.00 27.83 S
45	ATOM	2240		TIP	S	55	94.012	3.488	1.399	1.00 24.78 S
43					S	58				
	MOTA	2241	OH2	TIP			85.735		-18.436	
	MOTA	2242		TIP	S	61	79.069	-4.638	12.345	1.00 21.04 S
	MOTA	2243			S	64	103.981	17.563	-7.228	1.00 28.86 S
	MOTA	2244		TIP	S	66	79.020	43.119	5.431	1.00 33.30 S
50	ATOM	2245	OH2	TIP	s	69	88.177	36.956	3.079	1.00 30.87 S
	MOTA	2246	OH2	TIP	S	75	78.707	27.486	-3.439	1.00 25.25 S
	MOTA	2247	OH2	TIP	S	79	80.347	33.345	6.422	1.00 38.57 S
	ATOM	2248	OH2	TIP	S	84	64.594	19.493	24.406	1.00 26.01 S
	ATOM	2249		TIP	S	98	70.215	21.980	19.413	1.00 24.75 S
55	ATOM	2250		TIP	s	116	103.456	14.637	-2.925	1.00 41.84 S
	ATOM	2251	OH2	TIP	S	120	97.528		-14.706	1.00 43.27 S
	ATOM	2252	OH2	TIP	S	128	103.602	10.418	-1.388	1.00 37.07 S
	ATOM	2253		TIP		129	83.353	33.273	4.410	1.00 37.07 S
		2254	OH2	TIP		130	74.116	4.597	-3.022	1.00 34.76 S
	ATOM	4454	OH2	LIP	3	T20	/4.11b	4.09/	-3.022	1.00 27.69 5

	ATOM	2255	OH2	TIP	s	131	73.104	-1.689	21.760	1.00	32.76	S
	ATOM	2256	OH2	TIP	s	133	101.510	19.036	-1.083	1.00	28.30	S
	MOTA	2257	OH2	TIP	s	134	65.138	6.209	20.472	1.00	27.43	S
	ATOM	2258	OH2	TIP		135	94.509	36.623	-12.734	1.00	40.27	s
5	ATOM	2259	OH2	TIP		136	76.896		-17.698		37.17	s
	MOTA	2260	OH2	TIP		137	97.379	7.497	-6.673		41.53	s
	ATOM	2261	OH2	TIP		138	62,239	17.934	24.368		34.35	s
	ATOM	2262	OH2	TIP		139	69.630		-10.771		38.17	s
	ATOM	2263	OH2	TIP	s	140	84.554	44.493	-2.658		24.74	S
10	ATOM	2263	OH2	TIP		141	94.631	8.129	-9.752		35.45	S
10												
	ATOM	2265	OH2	TIP	S	142	78.415	1.021	3.883		28.60	S
	ATOM	2266	OH2		S	143	99.830		-10.148		35.79	S
	MOTA	2267	OH2	TIP		144	71.235	20.688	11.365		51.52	S
	ATOM	2268	OH2	TIP		145	87.138	25.623	11.165		41.92	S
15	MOTA	2269	OH2	TIP	S	146	60.803	15.332	23.294		32.69	S
	MOTA	2270	OH2		S	148	73.970		-13.455		33.99	S
	MOTA	2271	OH2	TIP	S	149	88.146	19.004	17.326		27.60	S
	MOTA	2272	OH2	TIP	s	150	90.803	9.970	18.127		35.03	S
	MOTA	2273	OH2	TIP	s	153	86.261	32.393	-16.403	1.00	41.89	S
20	MOTA	2274	OH2	TIP	s	155	102.147	7.767	-0.215	1.00	38.83	S
	ATOM	2275	OH2	TIP	s	159	95.238	0.811	-7.614	1.00	47.22	S
	MOTA	2276	OH2	TIP	S	163	92.356	36.543	-5.580	1.00	40.19	S
	ATOM	2277	OH2	TIP	s	172	66.640	4.633	22.314	1.00	29.95	S
	ATOM	2278	OH2	TIP	s	176	99.303	9.124	3.136	1.00	37.07	S
25	ATOM	2279	OH2	TIP	s	184	104.566	20.517	-7.318	1.00	40.83	S
	ATOM	2280	OH2	TIP		185	90.295		-15.433		34.81	S
	ATOM	2281	OH2	TIP		186	82.626	12.831	8.023		23.99	S
	ATOM	2282	OH2	TIP		187	86.159	18.737	24.618		32.12	S
	ATOM	2283	OH2	TIP		188	79.867	7.010	-7.877		28.52	s
30	ATOM	2284	OH2	TIP	s	189	88.469	4.967	1.404		45.39	S
50	ATOM	2285	OH2	TIP		190	95.628		-17.705		31.73	S
	ATOM	2286	OH2	TIP		191	76.228	7.822	28.547		36.76	S
	ATOM	2287	OH2			192	85.930	8.936	23.323		31.58	S
	ATOM	2288	OH2	TIP		193	73.669		-14.317		34.12	S
25												
35	ATOM	2289	OH2	TIP	S	194	99.847	12.959	4.319		43.06	S
	ATOM	2290	OH2	TIP	S	195	76.225	28.669	-3.386		38.83	S
	MOTA	2291	OH2	TIP		197	76.955	24.214	20.057		35.16	S
	MOTA	2292	OH2	TIP	S	198	65.723	11.313	28.926		38.40	S
	MOTA	2293	OH2	TIP		199	88.482	28.463	4.472		29.21	S
40	MOTA	2294	OH2	TIP		200	71.017		-13.980		37.15	S
	MOTA	2295	OH2	TIP	S	201	64.967	12.265	13.947		55.03	S
	MOTA	2296	OH2	TIP	S	204	99.611		-14.818		46.97	S
	MOTA	2297	OH2		S	205	65.422	-1.944	20.970		65.13	S
	MOTA	2298	OH2	TIP		210	89.648	5.683	12.672		38.65	S
45	ATOM	2299	OH2	TIP	S	213	80.842	40.555	7.721		37.38	S
	MOTA	2300	OH2	TIP	S	214	77.452	22.142	23.411	1.00	36.35	S
	ATOM	2301	OH2	TIP	S	216	104.280	21.111	-10.347	1.00	35.15	S
	MOTA	2302	OH2	TIP	S	225	84.900	44.787	-5.575	1.00	36.10	S
	MOTA	2303	OH2	TIP	S	230	74.759	19.808	9.165	1.00	29.67	S
50	ATOM	2304	OH2	TIP	s	231	76.375	2.991	-2.919	1.00	33.34	S
	MOTA	2305	OH2	TIP	s	232	97.252	36.990	-15.430	1.00	39.17	S
	ATOM	2306	OH2	TIP			70.180	4.692	8.907		29.97	S
	ATOM	2307	OH2	TIP			96.055	11.349	-8.926		29.40	s
	ATOM	2308	OH2			235	70.916	31.535	4.186		53.99	s
55	ATOM	2309	OH2	TIP		236	83.279	23.905	15.245		40.79	s
	ATOM	2310	OH2	TIP		237	90.441	34.500	3.752		37.91	S
	ATOM	2311	OH2	TIP	S	238	74.369		-11.954		36.85	S
	ATOM	2312	OH2			239	82.630	5.971	5.382		48.63	
	ATOM	2312	OH2				101.866	29.649	1.029		48.93	S
	ALUM	4313	OnZ	TIP	0	240	TOT. 999	49.049	1.029	1.00	20.23	۵

	MOTA	2314		GLC		2	74.980	15.310	28.834		58.25 G	
	MOTA	2315		GLC		2	74.113	15.072	27.724	1.00		
	MOTA	2316	C13	GLC	G	2	74.885	14.362	26.609	1.00		
	MOTA	2317	014	GLC	G	2	73.990	14.120	25.524	1.00	58.57 G	
5	ATOM	2318	C15	GLC	G	2	75.438	13.023	27.096	1.00	57.55 G	
	MOTA	2319	016	GLC	G	2	74.357	12.183	27.507	1.00	57.24 G	
	MOTA	2320	012	GLC	G	3	68.191	4.312	13.268	1.00	63.76 G	
	ATOM	2321	C11	GLC	G	3	67.998	3.273	14.231	1.00	63.57 G	
	ATOM	2322	C13	GLC	G	3	69.274	2.429	14.330	1.00	64.06 G	
10	ATOM	2323	014	GLC	G	3	69.570	1.858	13.049	1.00	62.75 G	
	ATOM	2324		GLC		3	69.094	1.303	15.364	1.00		
	ATOM	2325		GLC		3	68.010	0.444	14.978	1.00		
	ATOM	2326		GLC		4	87.921		-13.378	1.00		
	ATOM	2327		GLC	G	4	88.767		-14.265	1.00		
15	ATOM	2328		GLC		4	90.050		-13.526	1.00		
	ATOM	2329		GLC		4	90.660		-13.104	1.00		
	ATOM	2330		GLC		4	90.999		-14.435	1.00		
	ATOM	2331		GLC		4	92.193		-13.700	1.00		
	ATOM	2332		GLC	G	6	78.608	8.519	28.683	1.00		
20	ATOM	2332		GLC		6	79.227	8.721	29.956	1.00		
20	ATOM	2334		GLC		6	80.218	9.877	29.849	1.00		
	ATOM	2335		GLC	G	6	81.208	9.537	28.896	1.00		
	ATOM	2336		GLC	G	6	80.904	10.129	31.180	1.00		
2.5	MOTA	2337		GLC		6	81.611	8.950	31.564	1.00		
25	ATOM	2338		GLC		8	83.278	5.163	12.485	1.00		
	MOTA	2339		GLC		8	82.460	3.987	12.559	1.00		
	MOTA	2340		GLC	G	8	83.236	2.894	13.286	1.00		
	MOTA	2341		GLC		8	84.408	2.621	12.529	1.00		
	MOTA	2342		GLC		8	82.412	1.597	13.414	1.00		
30	MOTA	2343		GLC	G	8	82.051	1.062	12.130	1.00		
	MOTA	2344		GLC		10	87.146	4.682	-5.006	1.00		
	ATOM	2345		GLC		10	85.823	5.086	-5.356	1.00		
	MOTA	2346		GLC		10	85.782	5.498	-6.835		30.79 G	
	ATOM	2347		GLC		10	86.689	6.600	-7.069	1.00	29.47 G	
35	ATOM	2348		GLC		10	84.354	5.916	-7.219	1.00		
	ATOM	2349		GLC		10	83.947	7.022	-6.417	1.00		
	MOTA	2350	CBI	DRG	L	1	82.223	19.878	9.473	1.00	17.56 L	
	MOTA	2351	OBH	DRG	L	1	82.835	19.573	10.730	1.00	20.33 L	
	MOTA	2352	CBG	DRG	L	1	82.419	20.512	11.733	1.00	17.87 L	
40	ATOM	2353	CBF	DRG	L	1	83.661	21.291	12.177	1.00	16.47 L	
	ATOM	2354	NBK	DRG	L	1	84.171	22.133	11.085	1.00	15.68 L	
	MOTA	2355	CBJ	DRG	L	1	83.683	23.479	10.751	1.00	12.47 L	
	ATOM	2356	CBE	DRG	L	1	84.739	20.294	12.600	1.00	16.76 L	
	ATOM	2357	CBA	DRG	L	1	84.178	19.405	13.715	1.00	18.27 L	
45	ATOM	2358	OBB	DRG	L	1	82.790	19.632	14.017	1.00	18.03 L	
	ATOM	2359	CBC	DRG	L	1	81.853	19.747	12.937	1.00	18.62 L	
	ATOM	2360	CBD	DRG	L	1	80.732	20.611	13.524	1.00	14.59 L	
	ATOM	2361		DRG		1	81.398	18.547	12.551	1.00		
	ATOM	2362		DRG		1	80.185	18.344	12.014	1.00		
50	ATOM	2363		DRG		1	79.107	19.141	11.643	1.00		
	ATOM	2364		DRG		1	77.988	18.555	11.053	1.00		
	ATOM	2365		DRG		1	77.930	17.180	10.830	1.00		
	ATOM	2366		DRG		1	78.999	16.366	11.196	1.00		
	ATOM	2367		DRG		1	80.107	16.973	11.783	1.00		
55	ATOM	2368		DRG		1	81.290	16.377	12.187	1.00		
	ATOM	2369		DRG		1	81.811	15.087	12.083	1.00		
	ATOM	2370		DRG		1	82.083	17.407	12.657	1.00		
	ATOM	2371		DRG		1	83.404	17.144	13.014		18.70 L	
				DRG		1	84.365	17.144	13.438		17.82 L	
	MOTA	2372	NAT	DRG	ь	1	84.365	11.904	13.438	1.00	11.82 L	

	MOTA	2373	CAS	DRG	L	1	85.523	17.317	13.610	1.00 15.80 L
	MOTA	2374	CAR	DRG	L	1	86.807	17.682	14.000	1.00 14.23 L
	MOTA	2375	CAQ	DRG	L	1	87.803	16.708	14.047	1.00 13.92 L
	MOTA	2376	CAI	DRG	L	1	87.526	15.384	13.714	1.00 16.21 L
5	MOTA	2377	CAJ	DRG	L	1	86.244	15.003	13.324	1.00 16.43 L
	MOTA	2378		DRG		1	85.264	15.988	13,278	1.00 17.76 L
	MOTA	2379	CAL	DRG	L	1	83,932	15.867	12,904	1.00 18.99 L
	MOTA	2380	CAG	DRG	L	1	83.130	14.829	12.439	1.00 19.47 L
	MOTA	2381	CAC	DRG	L	1	83.403	13,472	12,290	1.00 18.70 L
10	MOTA	2382		DRG		1	84.471	12.895	12.480	1.00 18.10 L
	MOTA	2383		DRG		1	82,277	12.904	11.856	1.00 18.49 L
	MOTA	2384		DRG		1	81,128	13.799	11.622	1.00 20.08 L
	ATOM	2385		DRG		1	80.902	13.891	10.214	1.00 24.92 L
	MOTA	2386	S	SO4	I	1	64.638	8.174	16.414	1.00 89.13 I
15	MOTA	2387	01	SO4	I	1	65.311	9.465	16.666	1.00 88.78 I
	MOTA	2388	02	SO4	I	1	63.197	8.413	16.200	1.00 89.62 I
	MOTA	2389	03	SO4		1	64.827	7.262	17.566	1.00 88.49 I
	MOTA	2390	04	SO4	I	1	65.197	7.555	15.196	1.00 89.77 I
	MOTA	2391	S	SO4	I	3	84.884	-1.751	12.531	1.00 81.17 I
20	MOTA	2392	01	SO4	I	3	84.762	-0.302	12.775	1.00 81.32 I
	MOTA	2393	02	SO4	I	3	84.538	-2.490	13.758	1.00 81.49 I
	MOTA	2394	03	SO4	I	3	86,280	-2.053	12,162	1.00 81.73 I
	MOTA	2395	04	SO4	I	3	83.976	-2.163	11.440	1.00 81.19 I
	MOTA	2396	S	SO4	I	5	74.420	22.898	12.677	1.00 85.50 I
25	MOTA	2397	01	SO4	I	5	73.256	22.153	12.161	1.00 85.36 I
	MOTA	2398	02	SO4	I	5	75.637	22.104	12.412	1.00 84.51 I
	MOTA	2399	03	SO4	I	5	74.250	23.138	14.126	1.00 84.13 I
	MOTA	2400	04	SO4	I	5	74.527	24.202	11.997	1.00 85.44 I
	MOTA	2401	S	SO4	I	6	68.798	6.993	-3.457	1.00 73.84 I
30	MOTA	2402	01	SO4	I	6	68.338	7.338	-4.823	1.00 72.86 I
	MOTA	2403	02	SO4	I	6	69.298	8.206	-2.791	1.00 73.61 I
	MOTA	2404	03	SO4	I	6	69.888	6.003	-3.540	1.00 73.52 I
	MOTA	2405	04	SO4	I	6	67.690	6.426	-2.658	1.00 73.19 I
	MOTA	2406	02	PO4	P	100	66.501	25.721	2.616	1.00 85.98 P
35	MOTA	2407	03	PO4	P	100	64.376	25.028	1.654	1.00 86.96 P
	MOTA	2408	04	PO4	P	100	65.755	26.653	0.496	1.00 86.51 P
	MOTA	2409	01	PO4	P	100	64.621	27.279	2.570	1.00 86.98 P
	MOTA	2410	P	PO4	P	100	65.315	26.170	1.832	1.00 87.36 P
	MOTA	2411	S	SO4	Х	3	80.775	-0.045	7.874	0.50 22.29 X
40	MOTA	2412	01	SO4	Х	3	81.160	0.521	9.176	0.50 22.30 X
	MOTA	2413	02	SO4	Х	3	81.320	-1.407	7.778	0.50 22.49 X
	MOTA	2414	03	SO4	Х	3	81.309	0.781	6.777	0.50 23.26 X
	MOTA	2415	04	SO4	Х	3	79.305	-0.088	7.772	0.50 24.36 X
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